

Enhanced Ammonia Oxidation Catalysis by a Low-Spin Iron Complex Featuring *Cis* Coordination Sites

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S.1 General procedures

General Considerations: All manipulations were carried out using standard Schlenk or glovebox techniques under an N₂ or Ar atmosphere. Unless otherwise noted, solvents were deoxygenated and dried by thoroughly sparging with N₂ gas followed by passage through an activated alumina column in a solvent purification system (SG Water, USA LLC). For electrochemical measurements under an Ar atmosphere, solvents were further degassed and then left under Ar. All solvents were stored over activated 3 or 4 Å molecular sieves prior to use. Anhydrous ammonia gas was dried by passage through a calcium oxide drying tube. All reagents were purchased from commercial vendors and used without further purification unless otherwise stated. Tris(2-pyridylmethyl)amine (TPA),¹ tris(2-pyridylmethylamine) iron(II) triflate bis-acetonitrile ([TPAFe(MeCN)₂]OTf)₂,² 6-(1,1-di(pyridin-2-yl)ethyl)-2,2'-bipyridine (bpyPy₂Me),³ and 6-(1,1-di(pyridin-2-yl)ethyl)-2,2'-bipyridine iron(II) triflate bis-acetonitrile ([bpyPy₂MeFe(MeCN)₂]OTf)₂⁴ ¹⁵NH₄OTf was prepared from ¹⁵NH₄Cl (Cambridge Isotope Laboratories) by anion exchange with silver triflate or metathesis with triflic acid, followed by repeated recrystallization from boiling acetonitrile. ¹H NMR chemical shifts are reported in ppm relative to tetramethylsilane, using residual solvent resonances as internal standards.

Electrochemistry: Voltammetry experiments were carried out with a Biologic VSP-300 or CH Instruments 600B potentiostat using a one-compartment three-electrode cell, and coulometry experiments were carried out with a Biologic VSP-300 potentiostat using a one-compartment three-electrode cell with a septum capped 14/20 joint for headspace analysis. For voltammetry, a boron-doped diamond (BDD) working electrode (3 mm diameter), a Pt wire counter electrode, and a Ag/AgOTf reference electrode (5 mM AgOTf and 0.1 M TBAPF₆ in MeCN) were employed. For CPC, the same reference electrode was used, but a BDD plate (geometric area: 4 cm²) and a Pt mesh were used respectively as working and counter electrode. All redox potentials in the present work are reported versus the Fc/Fc⁺ couple, measured before each experiment to be approximately +0.12 V versus our Ag/AgOTf reference electrode.

CVs were collected at 100 mV·s⁻¹ unless specified otherwise. E_{1/2} values for the reversible waves were obtained from the half potential between the oxidative and reductive peaks. CV measurements were performed applying IR compensation, compensating 85% of the resistance measured at one high frequency value (100 kHz). Potential values for waves that are not fully reversible were obtained as the apparent standard potential from differential pulse voltammetry measurements

Gas Chromatography: Gas chromatography was performed in the Environmental Analysis Center using HP 5890 Series II instruments. Gas quantification was performed using a molecular sieve column attached to a thermal conductivity detector. Argon was the carrier gas. Standard curves were generated by direct injection of hydrogen or

nitrogen gas. Quantification of background nitrogen was determined using the background oxygen signal. Isotopic measurements were performed with a separate HP 5890 Series II equipped with a GasPro column using helium as the carrier gas.

NMR: NMR spectroscopy was performed using Varian and Bruker 400 MHz NMR spectrometers equipped with broadband auto-tune probes. ^1H NMR chemical shifts are reported in ppm relative to tetramethylsilane, using residual solvent resonances as internal standards.

UV-Vis: Spectra were collected using a Cary 60 instrument with Cary WinUV software.

X-ray Crystallography: XRD studies were carried out at the Beckman Institute Crystallography Facility on a Bruker D8 Venture diffractometer (Cu $K\alpha$ radiation). Structures were solved using direct methods with SHELXS or SHELXT and refined against F^2 on all data by full-matrix least squares with SHELXL.⁵ All of the solutions were performed in the Olex2 program.⁶ The crystals were mounted on a glass fiber under Paratone N oil.

X-ray Photoelectron Spectroscopy: XPS measurements were carried out in the Caltech Molecular Materials Resource Center using a Surface Science Instruments M-Probe ESCA spectrometer with the sample held at ultra-high vacuum ($< 2 \times 10^{-9}$ Torr), using the Al $K\alpha$ line at 1486.6 eV as a monochromatic X-ray source. XPS measurements were checked for surface charging effects, and the diamond carbon (sp^3) 1s peak was verified to be within ± 0.3 eV of 285 eV. A full scan from 0–1000 eV was acquired, and then scans at the binding energies typical for carbon (274–294 eV), boron (176–196 eV), nitrogen (389–409 eV), oxygen (522–542 eV), and iron (690–730 eV) were measured. For measurements of the BDD plate electrode after catalysis, the electrode was rinsed with acetonitrile and air dried prior to data collection.

S.2 NMR spectra for electronic structure elucidation

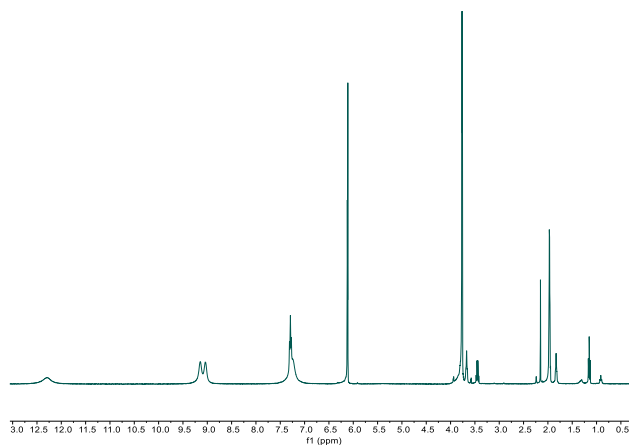


Figure S1. ^1H NMR spectrum of $[(\text{TPA})\text{Fe}(\text{MeCN})_2]\text{OTf}_2$ in CD_3CN at $25\text{ }^\circ\text{C}$. Spectrum also shows 1,3,5-trimethoxybenzene used for Evan's method.

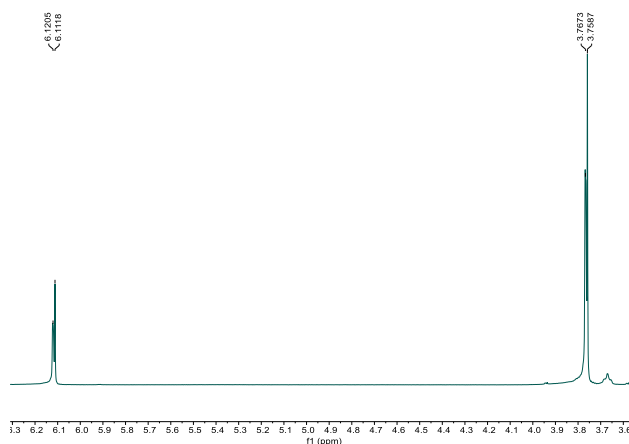


Figure S2. 1,3,5-trimethoxybenzene signals used for Evan's method for $[(\text{TPA})\text{Fe}(\text{MeCN})_2]\text{OTf}_2$ in CD_3CN at $25\text{ }^\circ\text{C}$. $[\text{Fe}] = 0.011\text{ M}$, $\Delta f = 3.46\text{ Hz}$, $f = 400.15\text{ MHz}$, $\mu = 0.68\mu\text{B}$.

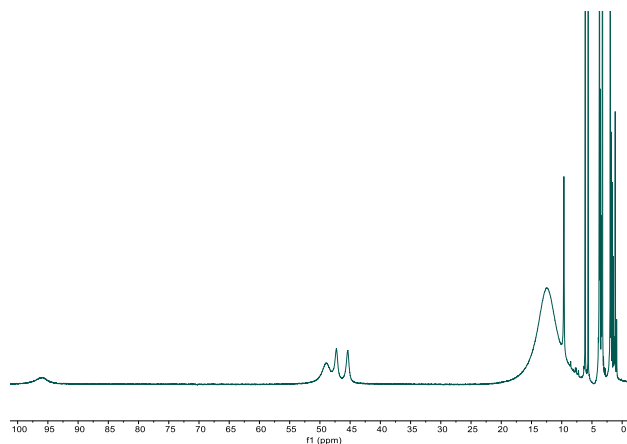


Figure S3. ^1H NMR spectrum of $[(\text{TPA})\text{Fe}(\text{L})_2]\text{OTf}_2$ ($\text{L} = \text{MeCN}, \text{NH}_3$) formed by mixing $[(\text{TPA})\text{Fe}(\text{MeCN})_2]\text{OTf}_2$ with 75 equivalents of NH_3 in CD_3CN at 25°C . Spectrum also shows 1,3,5-trimethoxybenzene used for Evan's method.

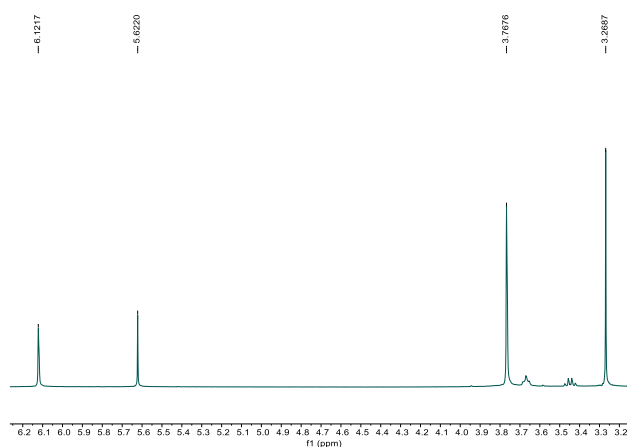


Figure S4. 1,3,5-trimethoxybenzene signals used for Evan's method for $[(\text{TPA})\text{Fe}(\text{L})_2]\text{OTf}_2$ ($\text{L} = \text{MeCN}, \text{NH}_3$), formed by mixing $[(\text{TPA})\text{Fe}(\text{MeCN})_2]\text{OTf}_2$ with 75 equivalents of NH_3 in CD_3CN at 25°C . $[\text{Fe}] = 0.011 \text{ M}$, $\Delta f = 200 \text{ Hz}$, $f = 400.15 \text{ MHz}$, $\mu = 5.2\mu\text{B}$.

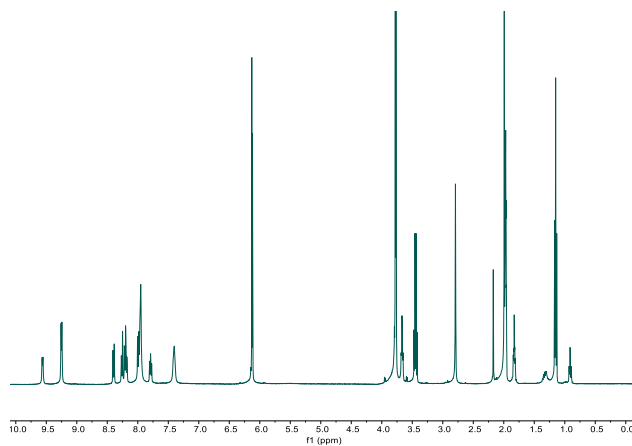


Figure S5. ^1H NMR spectrum of $[(\text{bpyPy}_2\text{Me})\text{Fe}(\text{MeCN})_2]\text{OTf}_2$ in CD_3CN at $25\text{ }^\circ\text{C}$. Spectrum also shows 1,3,5-trimethoxybenzene used for Evan's method.

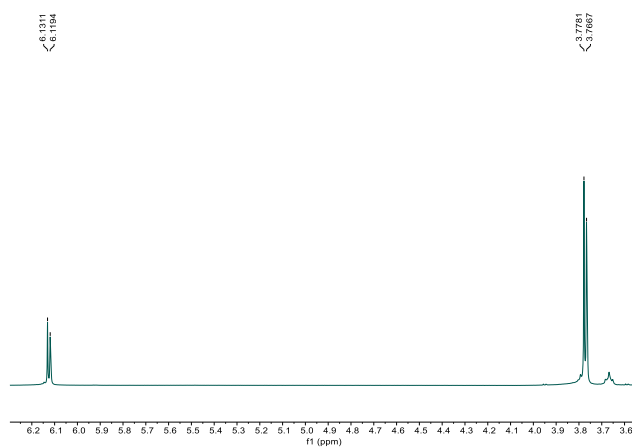


Figure S6. 1,3,5-trimethoxybenzene signals used for Evan's method for $[(\text{bpyPy}_2\text{Me})\text{Fe}(\text{MeCN})_2]\text{OTf}_2$ in CD_3CN at $25\text{ }^\circ\text{C}$. $[\text{Fe}] = 0.011\text{ M}$, $\Delta f = 4.62\text{ Hz}$, $f = 400.15\text{ MHz}$, $\mu = 0.79\mu\text{B}$.

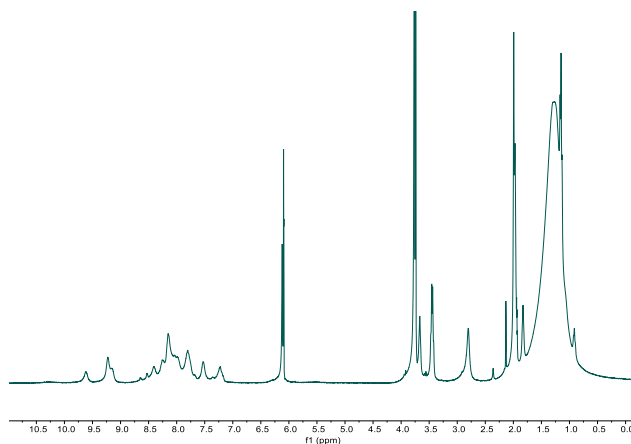


Figure S7. ^1H NMR spectrum of $[(\text{bpyPy}_2\text{Me})\text{Fe}(\text{L})_2]\text{OTf}_2$ ($\text{L} = \text{MeCN}, \text{NH}_3$) formed by mixing $[(\text{bpyPy}_2\text{Me})\text{Fe}(\text{MeCN})_2]\text{OTf}_2$ with 75 equivalents of NH_3 in CD_3CN at 25°C . Spectrum also shows 1,3,5-trimethoxybenzene used for Evan's method.

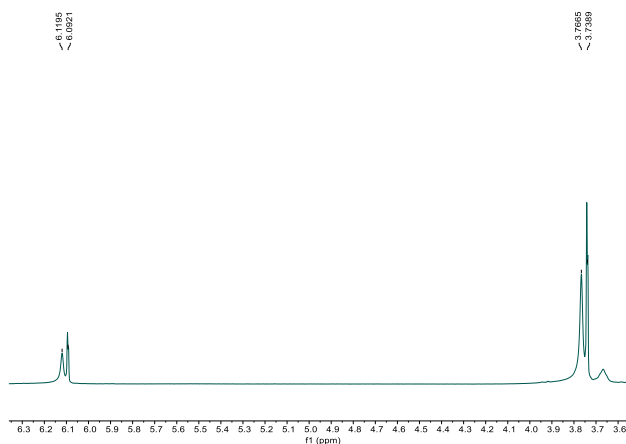


Figure S8. 1,3,5-trimethoxybenzene signals used for Evan's method for $[(\text{bpyPy}_2\text{Me})\text{Fe}(\text{L})_2]\text{OTf}_2$ ($\text{L} = \text{MeCN}, \text{NH}_3$), formed by mixing $[(\text{bpyPy}_2\text{Me})\text{Fe}(\text{MeCN})_2]\text{OTf}_2$ with 75 equivalents of NH_3 in CD_3CN at 25°C . $[\text{Fe}] = 0.011 \text{ M}$, $\Delta f = 11.0 \text{ Hz}$, $f = 400.15 \text{ MHz}$, $\mu = 1.2\mu_{\text{B}}$.

S.3 UV-vis spectra

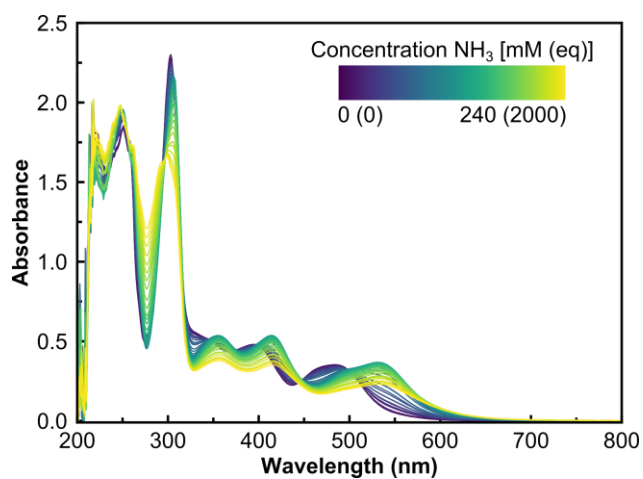


Figure S9. UV-vis spectra of acetonitrile solutions containing 0.12 mM $[(\text{bpyPy}_2\text{Me})\text{Fe}(\text{MeCN})_2]\text{OTf}_2$ and varying equivalents NH_3 in a 1 cm cuvette.

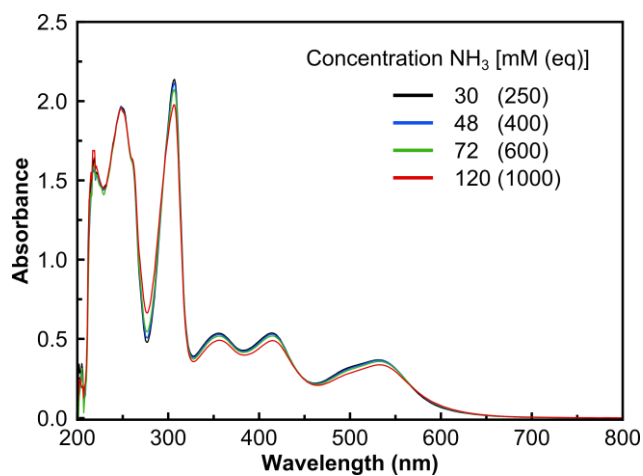


Figure S10. UV-vis spectra of acetonitrile solutions containing 0.12 mM $[(\text{bpyPy}_2\text{Me})\text{Fe}(\text{MeCN})_2]\text{OTf}_2$ with 250 (black), 400 (blue), 600 (green), or 1000 (red) equivalents NH_3 in a 1 cm cuvette. This shows the onset of demetallation around 600 equivalents NH_3 .

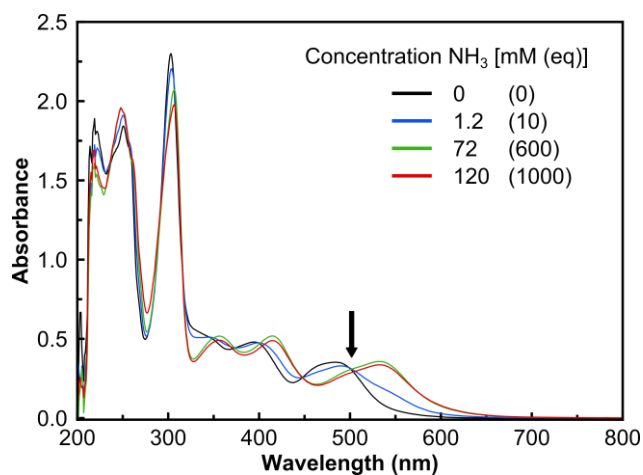


Figure S11. UV-vis spectra of acetonitrile solutions containing 0.12 mM $[(bpyPy_2Me)Fe(MeCN)_2]OTf_2$ with 0 (black), 10 (blue), 600 (green), or 1000 (red) equivalents NH_3 in a 1 cm cuvette. An arrow highlights an isosbestic point ~500 nm which is maintained for 0, 10, and 600 equivalents but has begun to show deviations assigned to demetallation at 1000 equivalents.

S.4 Catalytic controlled potential coulometry experiments

Procedures for controlled potential coulometry:

Preparation of the BDD electrode: A 10 cm² boron-doped diamond (BDD) plate electrode (IKA) was physically attached to standard electrical wire coated with chemical-resistant insulation, and the connection was covered with Teflon tape. The surface area of the electrode submerged in solution was around 4 cm².

BDD has a surface that exists in various states of reduction (H-terminated) and oxidation (O-terminated).⁷ In order to remove attached nitrogen and iron generated during controlled potential coulometry experiments and to ensure a reliable electrode surface prior to CPC measurements, the BDD plate electrode was oxidatively treated prior to use. First, the electrode was soaked in concentrated nitric acid for 5 minutes. Then, a potential of 3.0 V vs Ag/AgCl was applied to the BDD electrode in a 0.5 M H₂SO₄ solution for 10 minutes. The electrode was then thoroughly rinsed with water prior to use.

Preparation of the platinum counter electrode: In order to ensure a highly active Pt surface for hydrogen evolution prior to CPC experiments, the Pt mesh counter electrode was soaked in concentrated hydrochloric acid for at least 5 minutes prior to usage.

Preparation of the custom Ag/AgOTf reference electrode: To ensure reliable potential measurements, the custom Ag/AgOTf reference electrode was prepared prior to each CPC experiment and then a CV of ferrocene was measured. In a glass tube fitted with a Vycor porous glass frit attached by Teflon heatshrink tubing, an acetonitrile solution containing 5 mM AgOTf and 0.1 M TBAPF₆ was added. A silver wire was placed inside and the electrode was sealed.

Preparation of ammonia solutions. For experiments with natural abundance ammonia, saturated 2 M solutions⁸ in acetonitrile were prepared by bubbling anhydrous ammonia through acetonitrile in a Schlenk tube under an argon/ammonia atmosphere. For experiments with labeled ¹⁵NH₃, ammonia was liberated from ¹⁵NH₄OTf by addition of 1.1 equivalents of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) to ¹⁵N labeled ammonium triflate dissolved in acetonitrile in a Schlenk tube inside of an argon glovebox. This solution was then vacuum transferred to a separate, clean Schlenk tube.

CPC: Inside an argon glovebox, a gas-tight electrochemical cell equipped with a 24/40 cap containing three tungsten rods for electrical contacts and a valved 14/20 joint carefully sealed with a Suba-Seal septum was prepared. A BDD plate electrode (A = 4 cm²), high surface area platinum mesh electrode, and custom Ag/AgOTf reference electrode were connected to the 24/40 cap. All chemical reagents were then rapidly added to the cell to prevent evaporation of ammonia, and then, the cell was sealed with the 24/40 cap. Prior to each CPC experiment, a ZIR and CV were taken. No IR compensation was applied for CPC measurements. The CPC experiment was then conducted for 24 h. The cell was then removed from the glovebox for analysis by gas chromatography. For headspace

analysis, 100 μL of the headspace was injected into a GC-TCD for quantification using a lockable Hamilton syringe with a 26S gauge needle. For GC-MS, only 50 μL of the headspace was injected.

For each experiment, a 10 mL solution containing 0.05 mM [Fe], 20 mM NH_3 (1.0 mL of 0.2 M solution), and 50 mM NH_4OTf (84 mg) was prepared in acetonitrile.

Reload experiments: After a completed CPC experiment, the valved 14/20 joint on the electrochemical cell was sealed, the septum was removed, and a 14/20 joint-to-tubing adapter was connected. This joint was connected to a double-manifold Schlenk line and put under an argon atmosphere. Under a positive counter-flow of argon, the 24/40 electrode cap was removed and replaced with a ground-glass stopper. The cell was then carefully evaporated to dryness under vacuum and brought into an argon glovebox. To this cell containing ammonium triflate electrolyte and used catalyst was added 9 mL acetonitrile and 1.0 mL of a 0.2 M NH_3 solution to reset the ammonia concentration to the initial value. Then, the CPC experiment was performed following our standard procedures.

Table S1. Results of catalytic CPC experiments performed at 0.85 V vs Fc/Fc^+ for 24 h with 0.05 mM [Fe] and 20 mM NH_3 (400 equivalents). For entries where reload experiments were conducted, the entries are listed as x.1 and x.2 for the initial and subsequent reload experiment, respectively. LOQ indicates that the amount of gas produced was below the limit of quantification.

Entry	Fe Source	Eq. N_2	Charge (C)	FE N_2 (%)	FE H_2 (%)
1.1	$[(\text{bpyPy}_2\text{Me})\text{Fe}(\text{MeCN})_2]\text{OTf}_2$	89	29.9	86	77
2.1	$[(\text{bpyPy}_2\text{Me})\text{Fe}(\text{MeCN})_2]\text{OTf}_2$	83	26.5	91	80
3	$[(\text{bpyPy}_2\text{Me})\text{Fe}(\text{MeCN})_2]\text{OTf}_2$	97	31.1	91	93
4*	$[(\text{bpyPy}_2\text{Me})\text{Fe}(\text{MeCN})_2]\text{OTf}_2$	102	36.5	81	84
Avg. 1.1–4	$[(\text{bpyPy}_2\text{Me})\text{Fe}(\text{MeCN})_2]\text{OTf}_2$	93	–	87	84
1.2	$[(\text{bpyPy}_2\text{Me})\text{Fe}(\text{MeCN})_2]\text{OTf}_2$	55	21.1	77	78
2.2	$[(\text{bpyPy}_2\text{Me})\text{Fe}(\text{MeCN})_2]\text{OTf}_2$	57	19.7	84	67
Avg. Reload	$[(\text{bpyPy}_2\text{Me})\text{Fe}(\text{MeCN})_2]\text{OTf}_2$	56	–	81	73
3	None (NH_3 only)	LOQ	0.86	LOQ	73
4.1	$\text{FeOTf}_2 \cdot 2 \text{ MeCN}$	7.7	8.2	27	74
5	$\text{FeOTf}_2 \cdot 2 \text{ MeCN}$	7.1	7.5	28	33
Avg. 4.1–5	$\text{FeOTf}_2 \cdot 2 \text{ MeCN}$	7.4	–	28	54
4.2	$\text{FeOTf}_2 \cdot 2 \text{ MeCN}$	LOQ	1.2	LOQ	65

* Experiment performed with $^{15}\text{NH}_3$ and $^{15}\text{NH}_4\text{OTf}$

NMR spectra showing active catalyst after CPC:

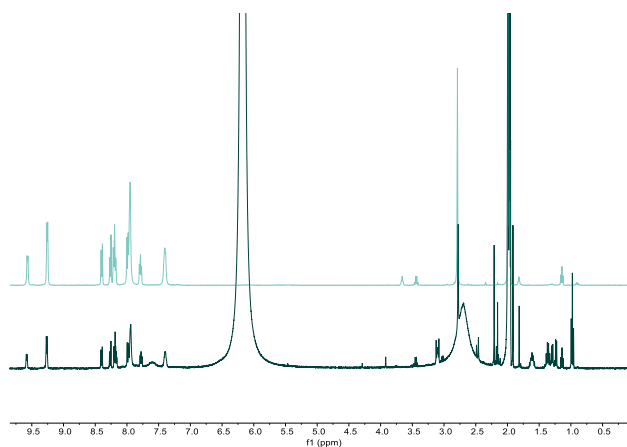


Figure S12. ^1H NMR spectra of $[(\text{bpyPy}_2\text{Me})\text{Fe}(\text{MeCN})_2]\text{OTf}_2$ precatalyst (top) and a sample extracted after a CPC experiment (bottom) in CD_3CN . The bottom spectrum shows that active catalyst remains after CPC experiments, as corroborated by reload experiments.

S.5 Electrode rinse test after CPC

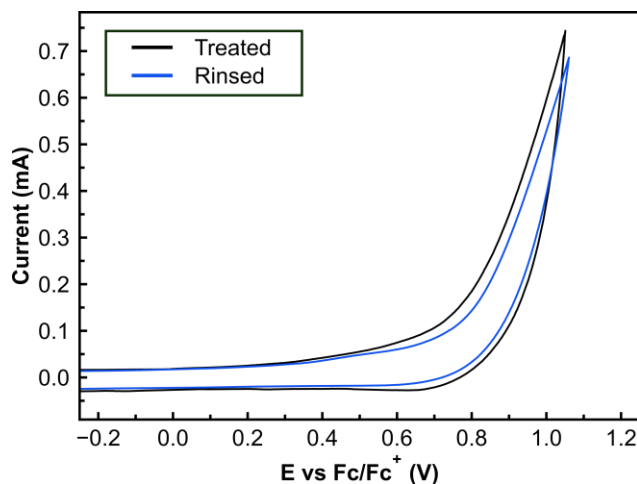


Figure S13. CVs of treated BDD plate electrode and the same electrode after CPC and rinsing with MeCN, recorded in MeCN with 0.05 M NH_4OTf and 20 mM NH_3 ; Pt counter and Ag/AgOTf reference electrodes. The rinsed electrode corresponds to the electrode after a 2 hour CPC experiment containing the new $[(\text{bpyPy}_2\text{Me})\text{Fe}(\text{MeCN})_2]\text{OTf}_2$ electrocatalyst under the optimized conditions detailed in Table S1. These measurements do not support the possibility of deposition of catalytically active material onto the electrode. This is in agreement with our previous investigation of the electrode after CPC with $[(\text{TPA})\text{Fe}(\text{MeCN})_2]\text{OTf}_2$.⁹

S.6 GC-MS data for $^{15}\text{NH}_3$ experiment

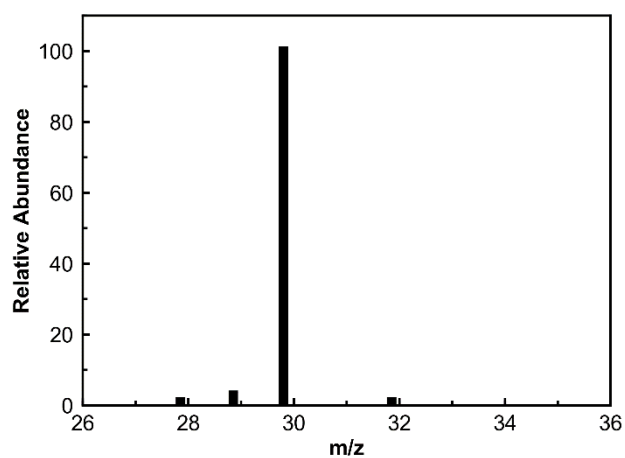


Figure S14. GC mass spectrum of headspace after CPC experiment using $^{15}\text{NH}_3$, showing $^{30}\text{N}_2$ as the major product.

S.7 XPS spectra of BDD plate electrode

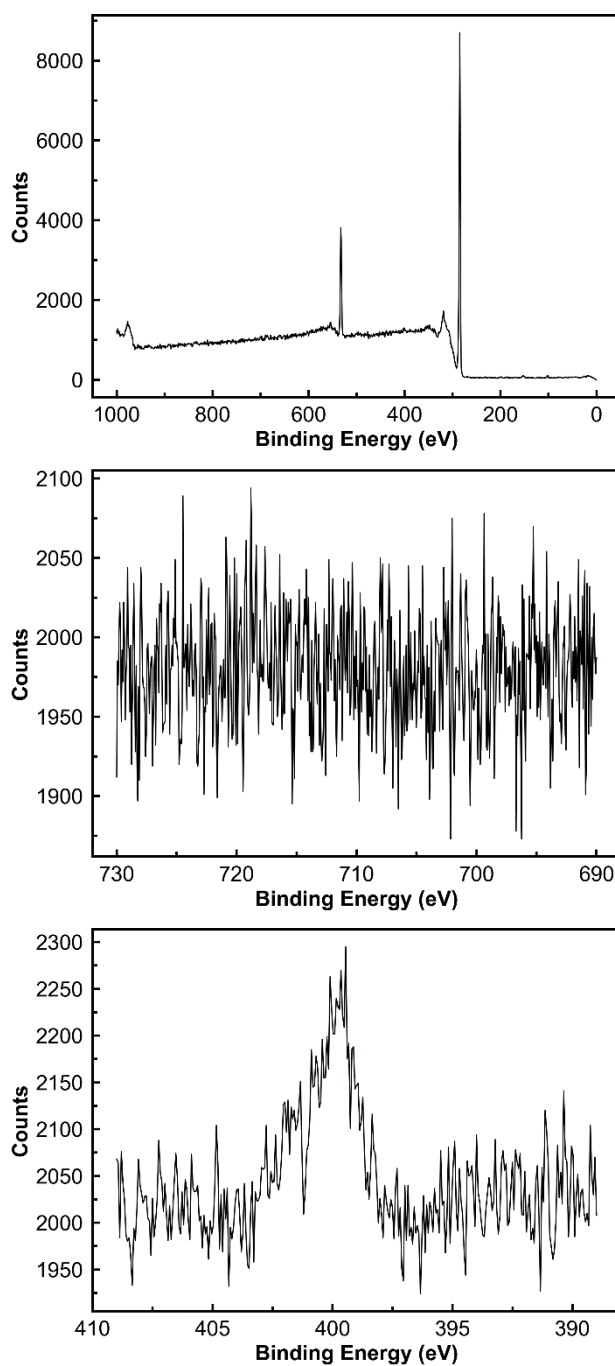


Figure S15. Full XPS spectrum of clean, treated BDD plate electrode and higher resolution spectra centered on the regions characteristic for Fe 2p and N 1s.

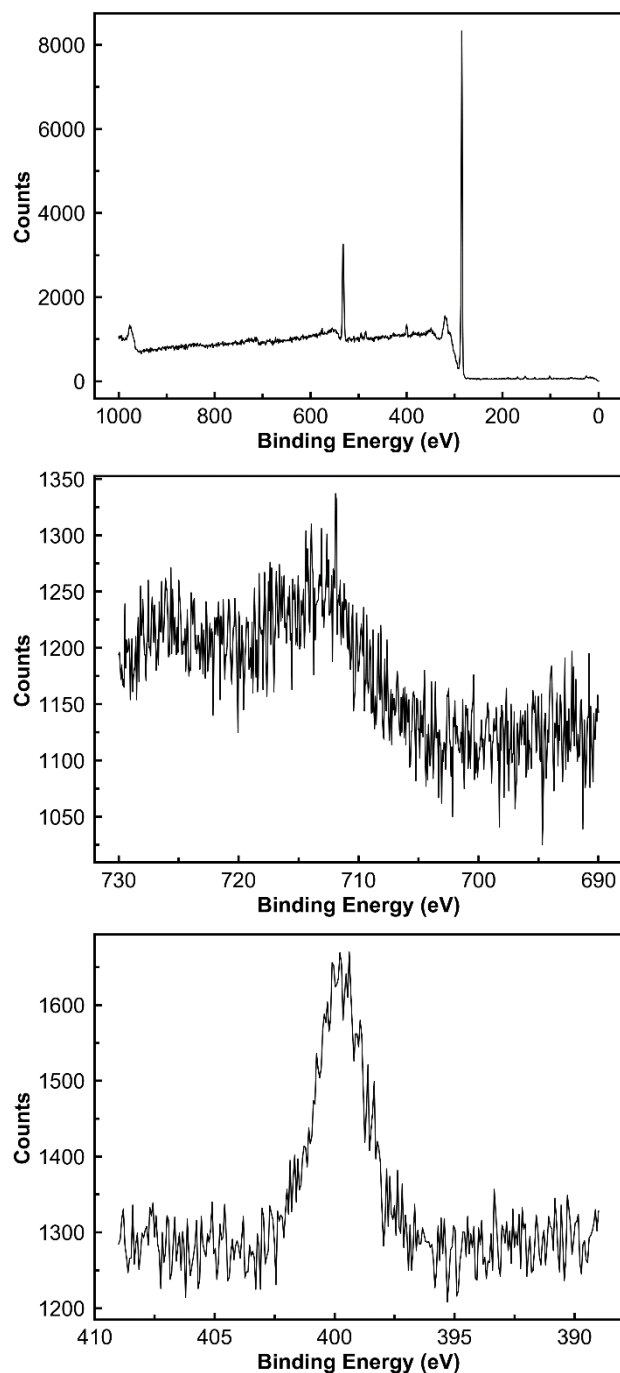


Figure S16. Full XPS spectrum of rinsed BDD plate electrode after 24 h CPC with 0.05 mM [(bpyPy₂Me)Fe(MeCN)₂]OTf₂ and 20 mM NH₃ solution and higher resolution spectra centered on the regions characteristic for Fe 2p and N 1s.

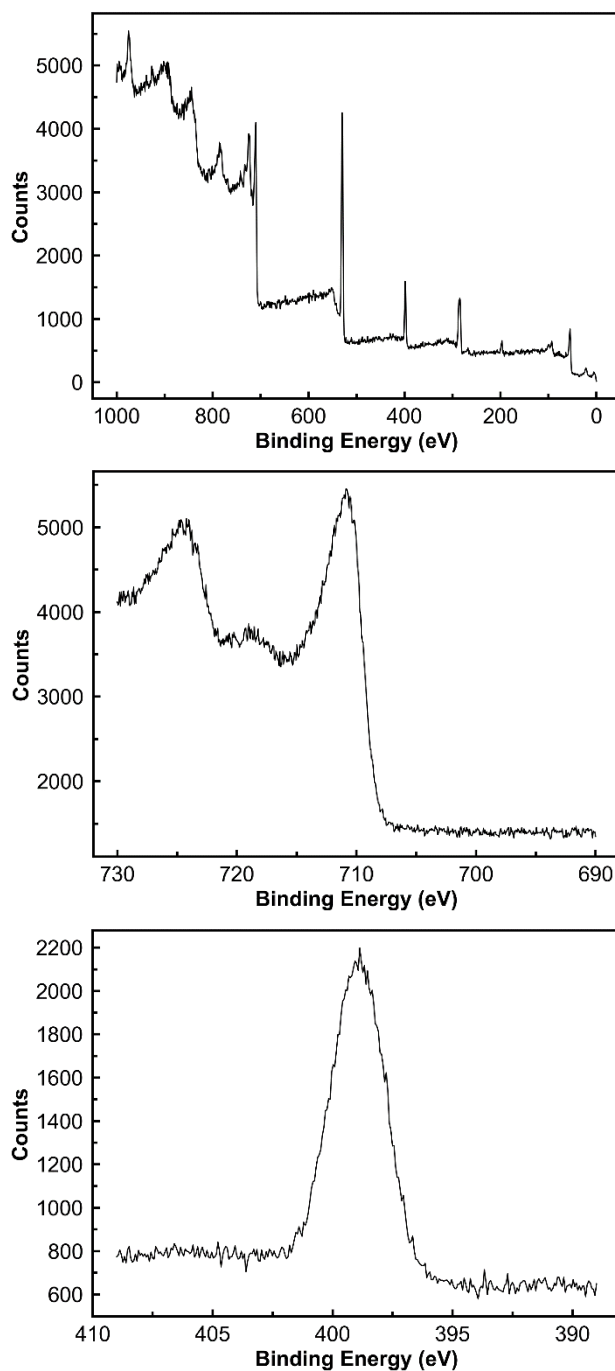


Figure S17. Full XPS spectrum of rinsed BDD plate electrode after 24 h CPC with 0.05 mM FeOTf₂ · 2 MeCN and 20 mM NH₃ solution and higher resolution spectra centered on the regions characteristic for Fe 2p and N 1s.

S.8 DPV data for E₁ analysis

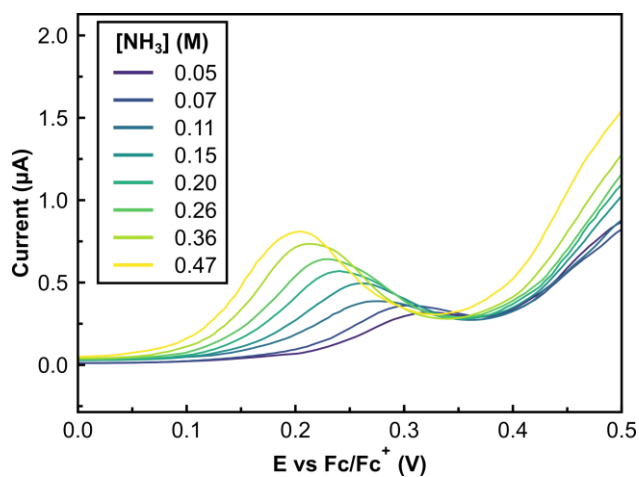


Figure S18. DPVs of 0.5 mM $[(bpyPy_2Me)Fe(MeCN)_2]OTf_2$ with varying NH_3 concentration in order to study the EC process at E₁. Recorded in MeCN with 0.05 M NH_4OTf using BDD working, Pt counter, and Ag/AgOTf reference electrodes.

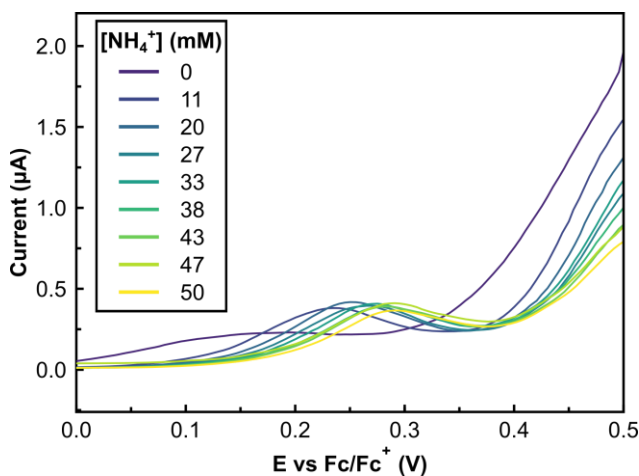


Figure S19. DPVs of 0.5 mM $[(bpyPy_2Me)Fe(MeCN)_2]OTf_2$ with varying NH_4^+ concentration in order to study the EC process at E₁. Recorded in MeCN with 0.2 M NH_3 and 0.1 M TBAPF₆ using BDD working, Pt counter, and Ag/AgOTf reference electrodes.

S.9 Further analysis of speciation related to E₁

In addition to the electrochemical and crystallographic data presented in the main text, we provide additional support for the assignment of the E₁ process here. We first further address the speciation at Fe(II), prior to E₁. The predominance of [(bpyPy₂Me)Fe(MeCN)(NH₃)]OTf₂ prior to E₁ in MeCN containing NH₃ is corroborated by SC-XRD (Fig. S20). From MeCN/NH₃ mixtures, [(bpyPy₂Me)Fe(MeCN)(NH₃)]OTf₂ can be isolated; alternatively, only [(bpyPy₂Me)Fe(NH₃)₂]OTf₂ has been crystallized in DCM/NH₃ mixtures containing 2 equivalents MeCN from the [(bpyPy₂Me)Fe(MeCN)₂]OTf₂ starting material. Isolation of the bis-ammine in DCM is compatible with DFT calculations which indicate a slight (3 kcal/mol) thermodynamic preference versus the mono-ammine; however, in MeCN solvent the large excess of MeCN relative to NH₃ likely favors the mono-acetonitrile adduct. Thus, [(bpyPy₂Me)Fe(MeCN)(NH₃)]OTf₂ is likely the primary iron species in bulk solution under our catalytic conditions.

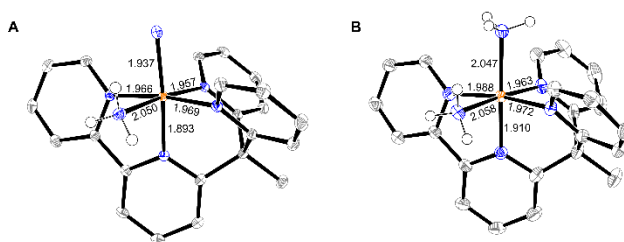


Figure S20. Solid-state crystal structure of **(A)** [(bpyPy₂Me)Fe(MeCN)(NH₃)]OTf₂ and **(B)** [(bpyPy₂Me)Fe(NH₃)₂]OTf₂ at 100 K, with select bond lengths labeled in angstroms. Thermal ellipsoids are shown at 50% probability. Triflate counterions and L_{aux} hydrogen atoms are omitted for clarity. The acetonitrile in **(A)** is truncated at nitrogen.

As mentioned in the main text, we have assigned the E₁ process to the proton-coupled oxidation of [(bpyPy₂Me)Fe(MeCN)(NH₃)]²⁺ to [(bpyPy₂Me)Fe(NH₂)(NH₃)]²⁺. This conclusion is in excellent agreement with our DFT results (Fig. S21) which show identical experimental and predicted potentials. However, two other likely pathways from [(bpyPy₂Me)Fe(MeCN)(NH₃)]²⁺ are proton-coupled oxidation without additional ammonia substitution (Scheme 2a in main text) or oxidation without proton transfer. Based on our DFT results, oxidation without proton transfer is the next lowest energy process, generating [(bpyPy₂Me)Fe(MeCN)(NH₃)]³⁺. The computed oxidation potential is 0.61 V, and we label this process E₁^{*}.

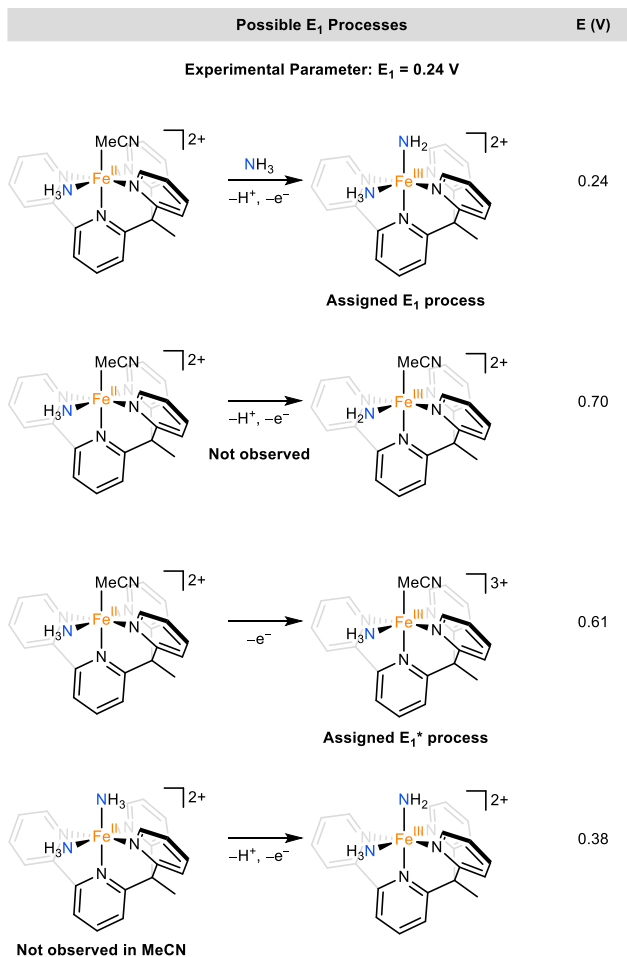


Figure S21. Possible E₁ processes and their calculated E (V) values.

When $[(bpyPy_2Me)Fe(MeCN)(NH_3)]^{2+}$ is investigated by CV at high scan rates under certain concentration regimes, an additional feature appears in the cyclic voltammogram as a shoulder in the catalytic E₂ wave at about 0.55 V (Fig. S22). This shoulder is minor at 200 mV/s but becomes clear at higher scan rates, e.g., 10000 mV/s. By DPV, this shoulder is more easily identified (Fig. S23). Given that the E₁ process, a proton-coupled oxidation associated with an additional ammonia substitution, could be slow due to the second order dependence on NH₃, it is unsurprising that this second feature can be observed. Interestingly, this shoulder does not move with varying NH₃ concentration as would be expected if it were also coupled to proton transfer. Furthermore, an increase in current at E₁* (Fig. S21, 2000 mV/s) results in an increase in return current at E₁, indicating that they are linked via a square mechanism, i.e., E₁ and E₁* generate the same product upon reduction. All of these data points agree with our assignment of E₁* as oxidation without proton transfer to generate $[(bpyPy_2Me)Fe(MeCN)(NH_3)]^{3+}$.

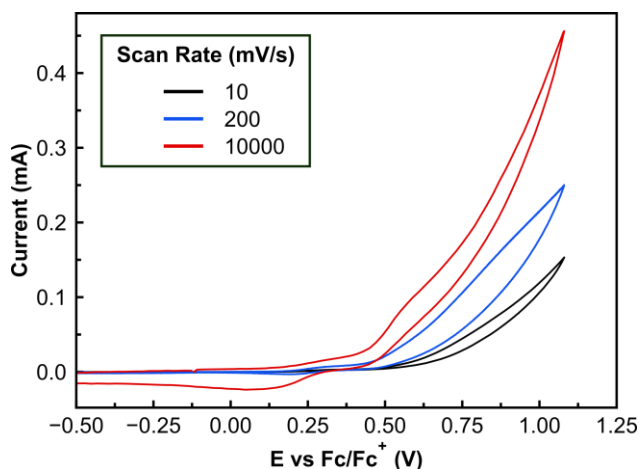


Figure S22. CVs of 0.5 mM [(bpyPy₂Me)Fe(MeCN)₂]OTf₂ with 0.2 M NH₃ at varying scan rates. Recorded in MeCN with 0.05 M NH₄OTf using BDD working, Pt counter, and Ag/AgOTf reference electrodes. The shoulder that appears at ~-0.55 V is discussed above.

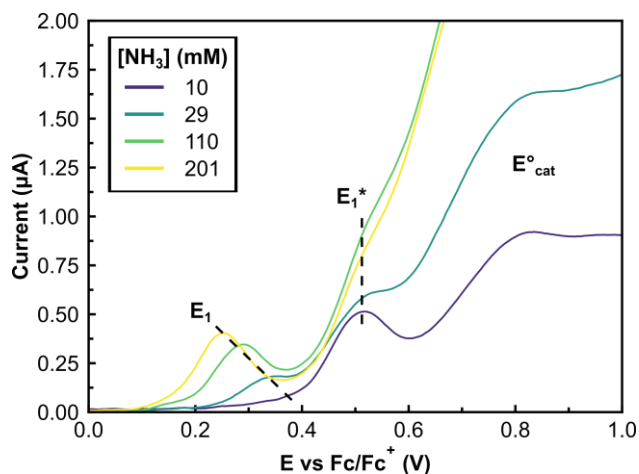


Figure S23. DPVs of 0.5 mM [(bpyPy₂Me)Fe(MeCN)₂]OTf₂ with varying NH₃ concentration in order to study the EC process at E₁. Recorded in MeCN with 0.05 M NH₄OTf using BDD working, Pt counter, and Ag/AgOTf reference electrodes. Labels highlight the E₁^{*} and E^o_{cat} processes discussed above.

S.10 Catalytic rate versus iron and NH₃ concentrations (E₂)

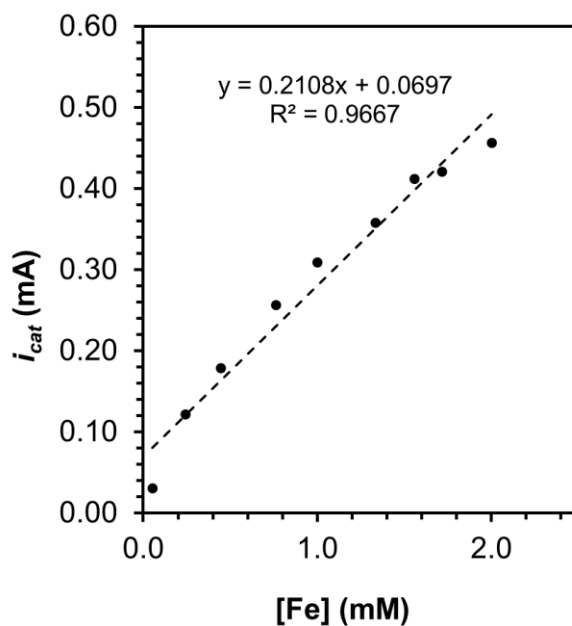


Figure S24. Rate dependence as measured by catalytic current at 1.08 V with varying concentrations of [(bpyPy₂Me)Fe(MeCN)₂]OTf₂ in MeCN with 0.05 M NH₄OTf and 0.2 M NH₃ with BDD working, Pt counter, and Ag/AgOTf reference electrodes.

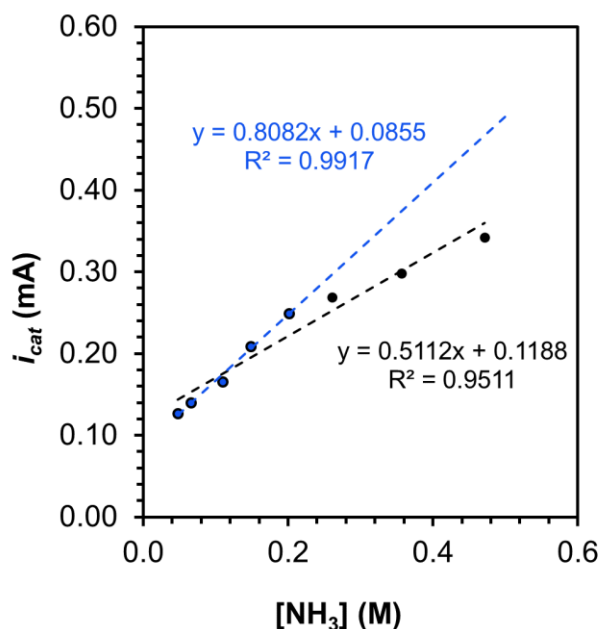


Figure S25. Rate dependence as measured by catalytic current at 1.08 V with varying concentrations of NH_3 and 0.5 mM $[(\text{bpyPy}_2\text{Me})\text{Fe}(\text{MeCN})_2]\text{OTf}_2$ in MeCN with 0.05 M NH_4OTf with BDD working, Pt counter, and Ag/AgOTf reference electrodes. The linear regression lines indicate a first-order dependence on $[\text{NH}_3]$. The low $[\text{NH}_3]$ regime is perfectly linear ($R^2 = 0.99$), but at higher concentrations the higher rate likely results in substrate depletion manifested by the mild concave behavior for the overall fit ($R^2 = 0.95$).

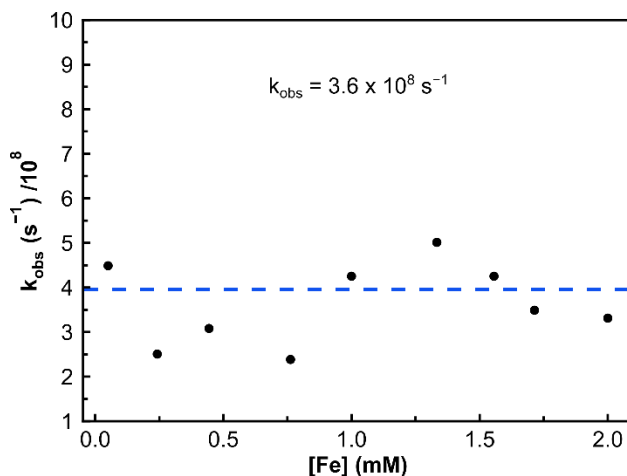


Figure S26. FOWA calculated k_{obs} for AO using varying concentrations of $[(\text{bpyPy}_2\text{Me})\text{Fe}(\text{MeCN})_2]\text{OTf}_2$ in MeCN with 0.05 M NH_4OTf and 0.2 M NH_3 with BDD working, Pt counter, and Ag/AgOTf reference electrodes. A first-order dependence on $[\text{Fe}]$ is incorporated into k_{obs} , thus the zero-order dependence of k_{obs} on $[\text{Fe}]$ in this plot indicates an overall first-order dependence on $[\text{Fe}]$.

S.11 Procedure for FOWA

Foot of the wave analysis was performed by using the equations deduced for EC_{cat} :

$$\frac{i}{i_p} = \frac{n \cdot 2.24 \cdot \sqrt{\frac{R \cdot T}{F \cdot v}} \cdot k_{obs}}{1 + \exp\left[\frac{F}{R \cdot T} (E^{\circ}_{cat} - E)\right]}$$

F is Faraday's constant, R is the gas constant, and T is the temperature. In this case, $n = 6$ due to the 6 electrons involved in ammonia oxidation to dinitrogen. The intensity of the one-electron wave (i_p) has been estimated from the one-electron oxidation precatalytic wave at E_1 for each condition. E°_{cat} was determined via differential pulse voltammetry. For each condition, the FOWA was performed in similar regions of the potential range in order to ensure a fair comparison. This region was selected as the foot-of-the-wave region where the plot of i/i_p versus $1/(1+\exp[F/(RT)(E^{\circ}_{cat}-E)])$ behaves linearly ($R^2 > 0.85$). Then, from the slope of that plot, the apparent pseudo-first order rate constant k_{obs} can be obtained and thus the value of the apparent second-order rate constant k'_{obs} . A representative example of this methodology is shown below for one condition.

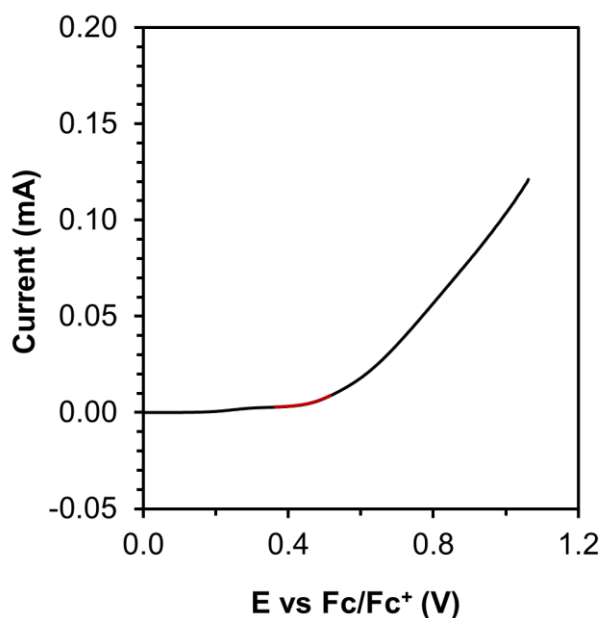


Figure S27. Linear sweep voltammogram with red trace showing the data range employed for performing the FOWA.

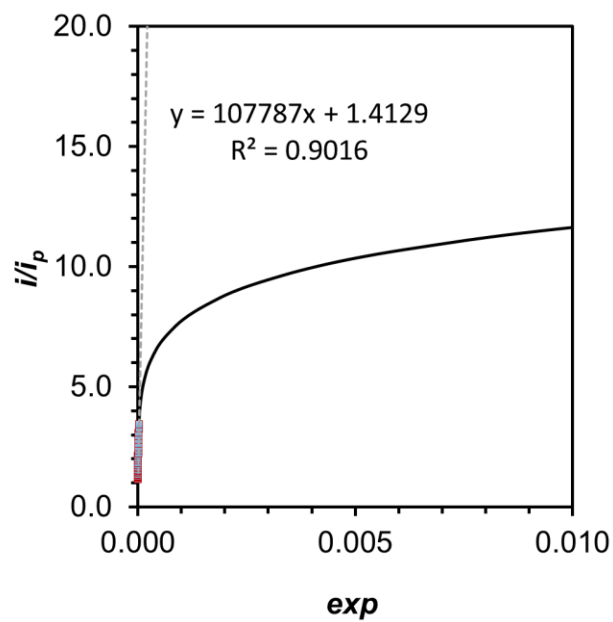


Figure S28. FOWA for an EC_{cat} mechanism calculated from the above linear sweep voltammogram showing strong concavity. The highlighted section and dotted line show the data employed for FOWA.

S.12 Further reactivity considered at E₂

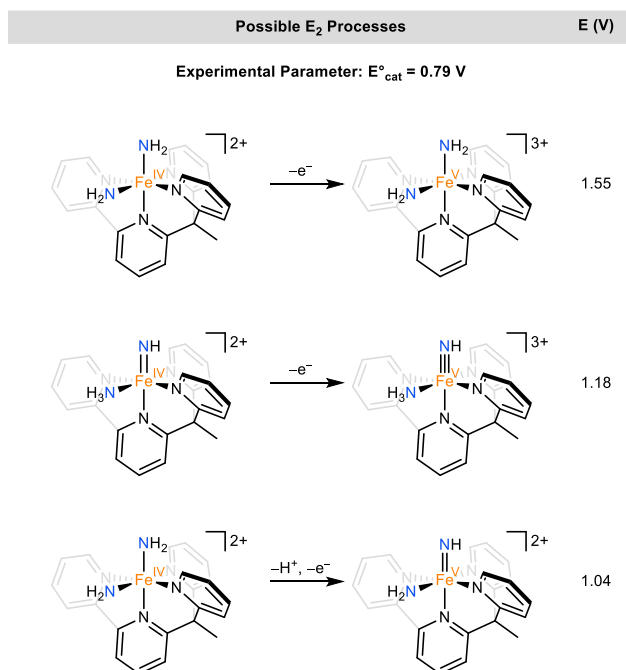


Figure S29. Further E₂ processes considered and their calculated E (V) values. All estimated E values are above the experimental E°_{cat} value. This data supports the hypothesis that N–N bond formation occurs after formation of the species presented in the main text, prior to further removal of protons and electrons.

S.13 Computational methodology

All computations were performed using the ORCA software package, version 4.0 or above.¹⁰ The DFT functional used was TPSS with the def2-SVP basis set for all atoms except iron, for which an augmented def2-TZVP basis set was used. An acetonitrile solvation model (conductor-like polarizable continuum model, CPCM) was used as implemented in ORCA. The RI-J approximation was used to speed up Coulomb integrals (as default). The convergence criteria employed were “tightscf” and “veryslowconv” as defined by ORCA. The Gibbs free energy at 298.15 K was computed in ORCA using harmonic vibrational frequencies computed numerically via “NumFreq”.

Sample input header:

```
! RI TPSS def2-SVP def2/J Opt NumFreq PAL8 tightscf veryslowconv
! CPCM(acetonitrile)
%basis
newgto Fe "def2-TZVP" end
end
```

To determine thermochemical values, oxidations are referenced to ferrocene/ferrocenium (Fc/Fc⁺), and reactions involving net hydrogen atom transfer are computed using TEMPO as a reference value (BDFE = 66.5 kcal/mol) and the acetonitrile C_G value of 54.9 kcal/mol.¹¹

For oxidations:



$E \text{ (V)} = \Delta G_{\text{ox}} / F$, where F (Faraday's constant) is in units of Hartree. 1 Hartree = 27.211 eV.

For reactions involving net hydrogen atom transfer:



$E \text{ (V)} = [\Delta G_{\text{BDFE}} - 54.9 + 66.5 - 1.37 \text{ pK}_a] / 23.06$, where ΔG_{BDFE} is in units of kcal/mol (1 Hartree = 627.51 kcal/mol). The pK_a is derived from that of NH_3 , 16.5 in MeCN,⁸ and adjusted by the Henderson–Hasselbalch equation to match the standard experimental CV conditions of 0.2 M NH_3 and 0.05 M NH_4^+ , resulting in $\text{pK}_a = 17.1$.

S.14 DFT spin-state ordering

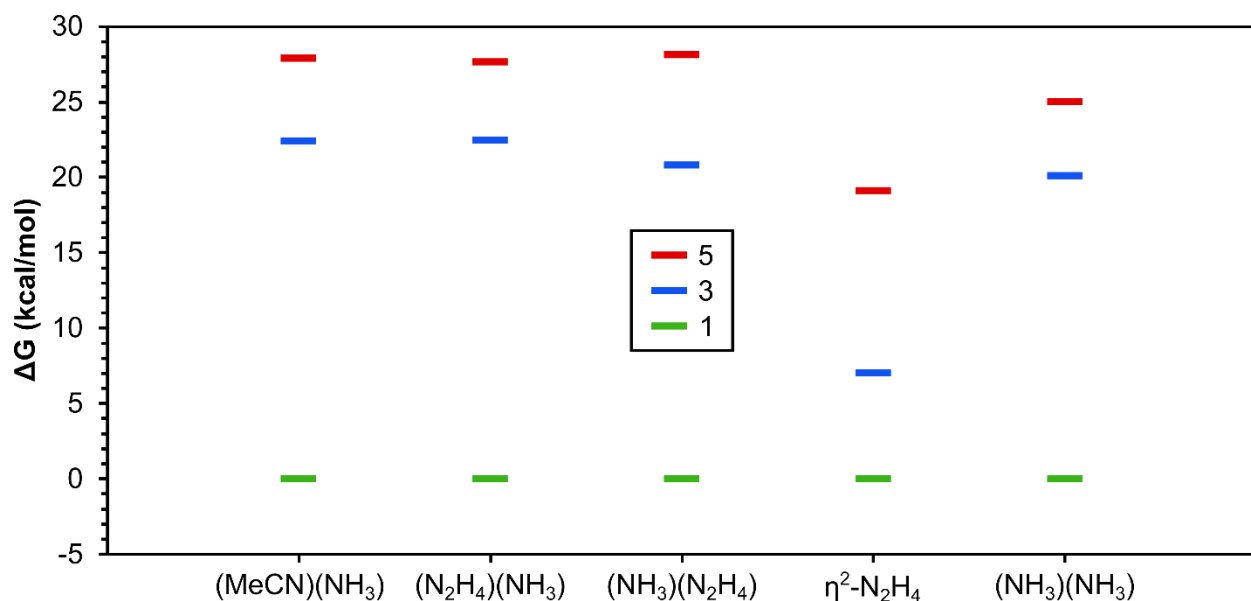


Figure S30. Relative energies for multiplicities of $[(\text{bpyPy}_2\text{Me})\text{Fe}(\text{L}_{\text{ax}})(\text{L}_{\text{eq}})]^{n+}$ complexes with formal oxidation states of +2. L_{ax} and L_{eq} represent ligands axial/*trans* to bipyridine and equatorial/*trans* to pyridine, respectively, in accordance with the orientation defined in the main-text. The lowest energy multiplicity is defined as 0.

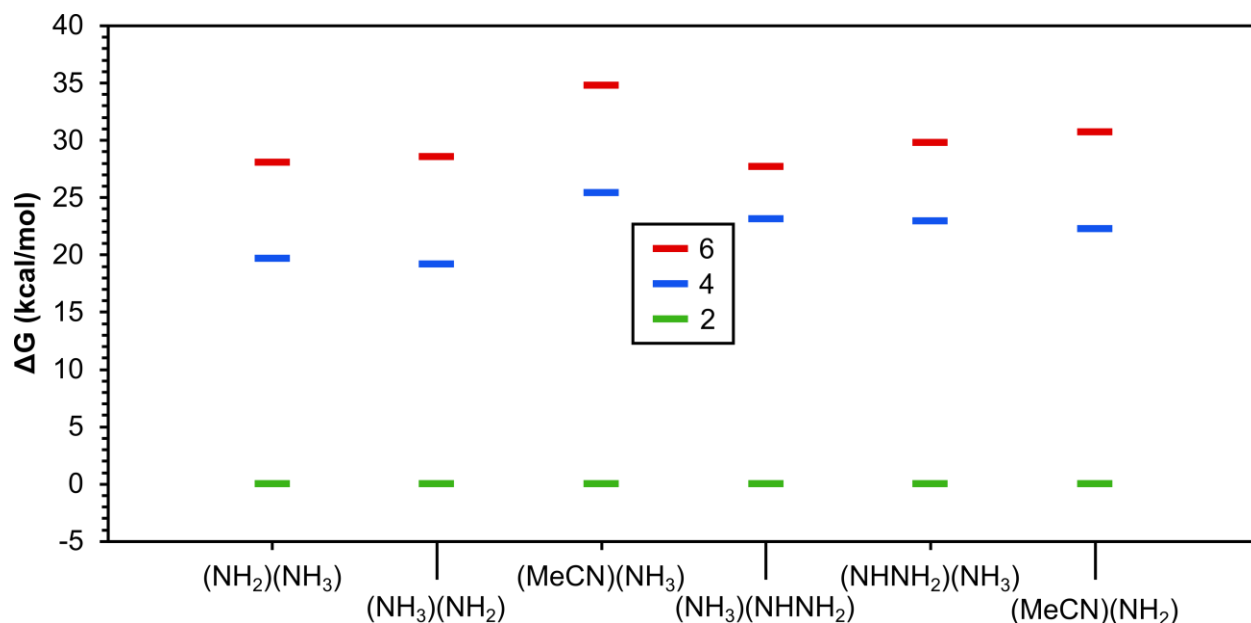


Figure S31. Relative energies for multiplicities of $[(\text{bpyPy}_2\text{Me})\text{Fe}(\text{L}_{\text{ax}})(\text{L}_{\text{eq}})]^{n+}$ complexes with formal oxidation states of +3. L_{ax} and L_{eq} represent ligands axial/*trans* to bipyridine and equatorial/*trans* to pyridine, respectively, in accordance with the orientation defined in the main-text. The lowest energy multiplicity is defined as 0.

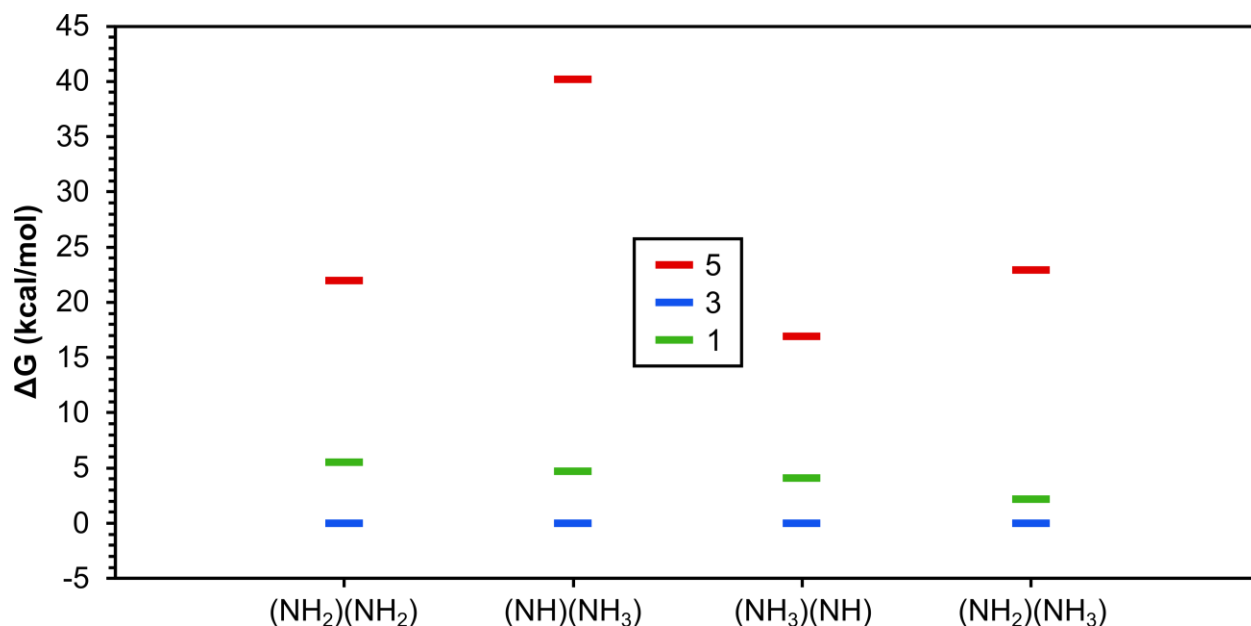


Figure S32. Relative energies for multiplicities of $[(\text{bpyPy}_2\text{Me})\text{Fe}(\text{L}_{\text{ax}})(\text{L}_{\text{eq}})]^{n+}$ complexes with formal oxidation states of +4. L_{ax} and L_{eq} represent ligands axial/*trans* to bipyridine and equatorial/*trans* to pyridine, respectively, in accordance with the orientation defined in the main-text. The lowest energy multiplicity is defined as 0.

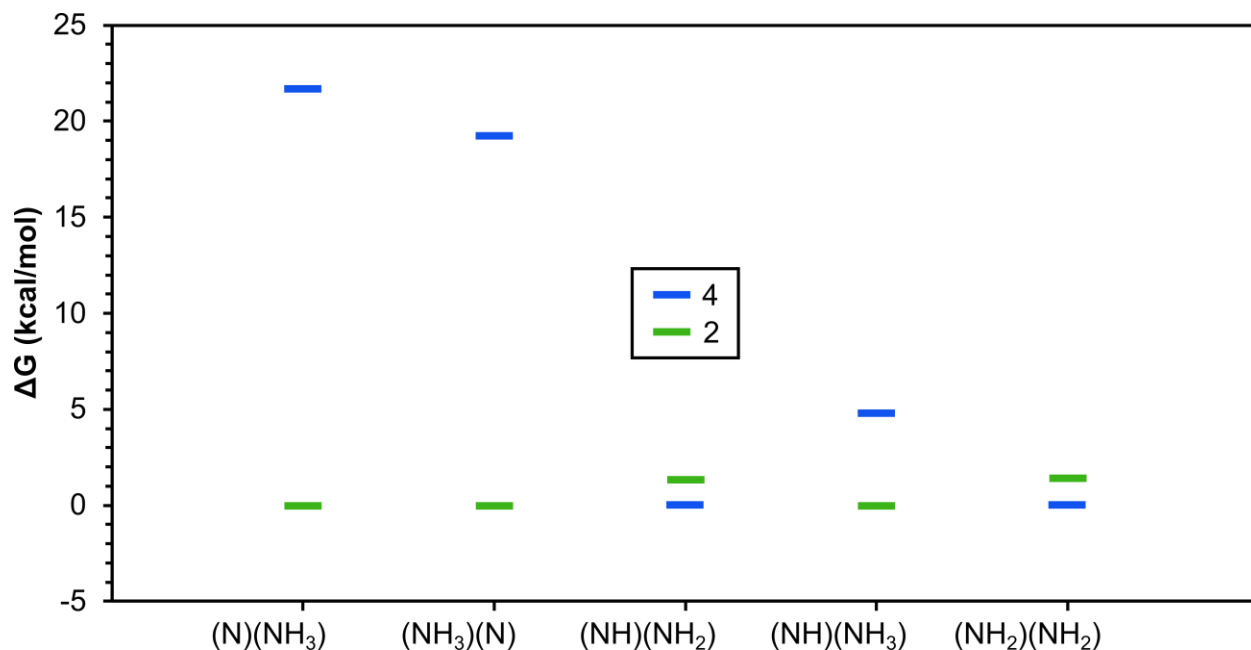


Figure S33. Relative energies for multiplicities of $[(\text{bpyPy}_2\text{Me})\text{Fe}(\text{L}_{\text{ax}})(\text{L}_{\text{eq}})]^{n+}$ complexes with formal oxidation states of +5. L_{ax} and L_{eq} represent ligands axial/*trans* to bipyridine and equatorial/*trans* to pyridine, respectively, in accordance with the orientation defined in the main-text. The lowest energy multiplicity is defined as 0.

S.15 DFT tabulated energies

Table S2. Gibbs free energy, oxidation state (O.S.), charge, and multiplicity for each compound studied in this work. The naming convention for $[(\text{bpyPy}_2\text{Me})\text{Fe}(\text{L}_{\text{ax}})(\text{L}_{\text{eq}})]^{n+}$, where L_{ax} and L_{eq} represent ligands axial/*trans* to bipyridine and equatorial/*trans* to pyridine, respectively, in accordance with the orientation defined in the main-text, is $\text{Fe}(\text{L}_{\text{ax}})(\text{L}_{\text{eq}})$.

Compound	O.S.	Charge	Multiplicity	Gibbs Free Energy (E_{h})
$\text{Fe}(\text{MeCN})(\text{NH}_3)$	2	2	1	-2520.170506
$\text{Fe}(\text{MeCN})(\text{NH}_3)$	2	2	3	-2520.134781
$\text{Fe}(\text{MeCN})(\text{NH}_3)$	2	2	5	-2520.126099
$\text{Fe}(\text{N}_2\text{H}_4)(\text{NH}_3)$	2	2	1	-2499.275282
$\text{Fe}(\text{N}_2\text{H}_4)(\text{NH}_3)$	2	2	3	-2499.239539
$\text{Fe}(\text{N}_2\text{H}_4)(\text{NH}_3)$	2	2	5	-2499.231216
$\text{Fe}(\text{NH}_3)(\text{N}_2\text{H}_4)$	2	2	1	-2499.280876
$\text{Fe}(\text{NH}_3)(\text{N}_2\text{H}_4)$	2	2	3	-2499.247766
$\text{Fe}(\text{NH}_3)(\text{N}_2\text{H}_4)$	2	2	5	-2499.236084
$\text{Fe}(\eta^2\text{-N}_2\text{H}_4)$	2	2	1	-2442.758364
$\text{Fe}(\eta^1\text{-N}_2\text{H}_4)^*$	2	2	3	-2442.747149
$\text{Fe}(\eta^1\text{-N}_2\text{H}_4)^*$	2	2	5	-2442.727913
$\text{Fe}(\text{NH}_3)_2$	2	2	1	-2444.013227
$\text{Fe}(\text{NH}_3)_2$	2	2	3	-2443.981207
$\text{Fe}(\text{NH}_3)_2$	2	2	5	-2443.973412
$\text{Fe}(\text{NH}_2)(\text{NH}_3)$	3	2	2	-2443.388803
$\text{Fe}(\text{NH}_2)(\text{NH}_3)$	3	2	4	-2443.357443
$\text{Fe}(\text{NH}_2)(\text{NH}_3)$	3	2	6	-2443.34405
$\text{Fe}(\text{NH}_3)(\text{NH}_2)$	3	2	2	-2443.383476
$\text{Fe}(\text{NH}_3)(\text{NH}_2)$	3	2	4	-2443.352874
$\text{Fe}(\text{NH}_3)(\text{NH}_2)$	3	2	6	-2443.337927
$\text{Fe}(\text{MeCN})(\text{NH}_3)$	3	3	2	-2519.973567
$\text{Fe}(\text{MeCN})(\text{NH}_3)$	3	3	4	-2519.933032
$\text{Fe}(\text{MeCN})(\text{NH}_3)$	3	3	6	-2519.918134
$\text{Fe}(\text{NH}_3)(\text{NHNH}_2)$	3	2	2	-2498.67244
$\text{Fe}(\text{NH}_3)(\text{NHNH}_2)$	3	2	4	-2498.635561
$\text{Fe}(\text{NH}_3)(\text{NHNH}_2)$	3	2	6	-2498.628327
$\text{Fe}(\text{NHNH}_2)(\text{NH}_3)$	3	2	2	-2498.676109
$\text{Fe}(\text{NHNH}_2)(\text{NH}_3)$	3	2	4	-2498.639554
$\text{Fe}(\text{NHNH}_2)(\text{NH}_3)$	3	2	6	-2498.628596
$\text{Fe}(\text{MeCN})(\text{NH}_2)$	3	2	2	-2519.534136
$\text{Fe}(\text{MeCN})(\text{NH}_2)$	3	2	4	-2519.498649
$\text{Fe}(\text{MeCN})(\text{NH}_2)$	3	2	6	-2519.48518
$\text{Fe}(\text{NH}_2)(\text{NH}_2)$	4	2	3	-2442.748256
$\text{Fe}(\text{NH}_2)(\text{NH}_2)$	4	2	1	-2442.739497

Compound	O.S.	Charge	Multiplicity	Gibbs Free Energy (E _h)
Fe(NH ₂)(NH ₂)	4	2	5	-2442.713299
Fe(NH)(NH ₃)	4	2	3	-2442.74475
Fe(NH)(NH ₃)	4	2	1	-2442.737322
Fe(NH)(NH ₃)	4	2	5	-2442.680746
Fe(NH ₃)(NH)	4	2	3	-2442.734741
Fe(NH ₃)(NH)	4	2	1	-2442.72829
Fe(NH ₃)(NH)	4	2	5	-2442.707865
Fe(NH ₂)(NH ₃)	4	3	3	-2443.173804
Fe(NH ₂)(NH ₃)	4	3	1	-2443.170371
Fe(NH ₂)(NH ₃)	4	3	5	-2443.137346
Fe(N)(NH ₃)	5	2	2	-2442.125412
Fe(N)(NH ₃)	5	2	4	-2442.090902
Fe(NH ₃)(N)	5	2	2	-2442.11944
Fe(NH ₃)(N)	5	2	4	-2442.088784
Fe(NH)(NH ₂)	5	2	4	-2442.099408
Fe(NH)(NH ₂)	5	2	2	-2442.097272
Fe(NH)(NH ₃)	5	3	2	-2442.526792
Fe(NH)(NH ₃)	5	3	4	-2442.519145
Fe(NH ₂)(NH ₂)	5	3	4	-2442.516784
Fe(NH ₂)(NH ₂)	5	3	2	-2442.514531
MeCN	—	0	1	-132.6671601
NH ₃	—	0	1	-56.50501517
N ₂ H ₄	—	0	1	-111.7692421
Ferrocene	2	0	1	-1650.613945
Ferrocenium	3	1	2	-1650.439308
TEMPO	—	0	2	-483.24406649
TEMPOH	—	0	1	-483.83585272

* For Fe(N₂H₄), calculations with multiplicities of 3 or 5 resulted in optimized geometries containing η¹-N₂H₄ moieties; η²-N₂H₄ coordination was only observed for the lowest energy singlet state.

S.16 DFT structures

Cartesian coordinates in angstrom units are provided. The naming convention is [(bpyPy₂Me)Fe(L_{ax})(L_{eq})]ⁿ⁺, where L_{ax} and L_{eq} represent ligands axial/*trans* to bipyridine and equatorial/*trans* to pyridine, respectively, in accordance with the orientation defined in the main-text.

[(bpyPy₂Me)Fe(MeCN)(NH₃)]²⁺, multiplicity = 1

C -2.5812420000 2.1854410000 -0.9943090000
C -3.0217660000 0.8802290000 -0.7505960000
C -2.0629920000 -0.1136280000 -0.5108580000
N -0.7289330000 0.1718060000 -0.5950930000
C -0.2977210000 1.4502580000 -0.6623920000
C -1.2134820000 2.4865760000 -0.8951380000
C -3.5780150000 -2.0225160000 0.2320770000
C -2.3105100000 -1.4688140000 -0.0023780000
C -3.6734330000 -3.2780260000 0.8408120000
C -2.4942460000 -3.9450220000 1.2012940000
C -1.2610950000 -3.3495070000 0.9214680000
N -1.1564730000 -2.1402770000 0.3264780000
C 1.1970940000 1.6469490000 -0.3363680000
C 1.5351780000 3.1453320000 -0.2748940000
C 2.0661280000 0.9212210000 -1.3777610000
C 1.4461390000 0.9552330000 1.0342530000
N 1.1544700000 -0.3733690000 1.1334160000
C 1.3453510000 -1.0144660000 2.3113780000
C 1.8462000000 -0.3726350000 3.4428090000
C 2.1614110000 0.9876660000 3.3544860000
C 1.9557160000 1.6528890000 2.1400560000
C 3.0282510000 1.5819880000 -2.1571800000
C 3.8083240000 0.8578870000 -3.0658040000
C 3.6113300000 -0.5236210000 -3.1683230000
C 2.6406570000 -1.1208780000 -2.3661030000
N 1.8728370000 -0.4188090000 -1.4921070000
H -3.3027470000 2.9809780000 -1.2012290000
H -4.6524710000 -3.7255750000 1.0338840000
H -2.5173130000 -4.9241040000 1.6862270000
H -0.3246170000 -3.8545620000 1.1679380000
H 0.9171690000 3.6524760000 0.4812650000
H 2.5936540000 3.2996290000 -0.0173040000
H 1.3459720000 3.6226960000 -1.2486520000
H 1.0817780000 -2.0748540000 2.3319930000
H 1.9826380000 -0.9378570000 4.3688070000
H 2.5602980000 1.5301510000 4.2168980000

H 2.1956700000 2.7136940000 2.0594060000
 H 3.1720610000 2.6584090000 -2.0561060000
 H 4.5587950000 1.3686600000 -3.6767970000
 H 4.1975990000 -1.1415180000 -3.8541250000
 H 2.4634050000 -2.1979560000 -2.4119290000
 Fe 0.4571770000 -1.3049970000 -0.4451370000
 H -0.8754380000 3.5195090000 -0.9871880000
 N 1.5623420000 -2.8147330000 -0.1573420000
 N -0.2218100000 -2.1161660000 -2.1835550000
 H -1.2230990000 -1.9408650000 -2.3488320000
 H -0.1113430000 -3.1381050000 -2.2216850000
 H 0.2538100000 -1.7453880000 -3.0160680000
 H -4.4765270000 -1.4701800000 -0.0537390000
 H -4.0881310000 0.6442440000 -0.7153050000
 C 2.2675500000 -3.7299440000 0.0181330000
 C 3.1447560000 -4.8685140000 0.2448010000
 H 3.1314360000 -5.1387990000 1.3141690000
 H 4.1753420000 -4.6094880000 -0.0521240000
 H 2.7994910000 -5.7290660000 -0.3521540000

[(bpyPy₂Me)Fe(MeCN)(NH₃)]²⁺, multiplicity = 3

C -2.5824880000 2.1460730000 -0.9169440000
 C -3.0324110000 0.8471120000 -0.6690650000
 C -2.0863310000 -0.1507490000 -0.4025140000
 N -0.7419370000 0.1224020000 -0.4351310000
 C -0.2987770000 1.3998360000 -0.5541770000
 C -1.2130030000 2.4311930000 -0.8206540000
 C -3.6840890000 -2.0375660000 0.2040690000
 C -2.3912740000 -1.5215580000 0.0178920000
 C -3.8329320000 -3.3374540000 0.6962860000
 C -2.6873640000 -4.0923620000 0.9901690000
 C -1.4298680000 -3.5283890000 0.7635690000
 N -1.2784660000 -2.2736220000 0.2866340000
 C 1.2048740000 1.6561840000 -0.2965590000
 C 1.4938760000 3.1680460000 -0.3206260000
 C 2.0742640000 0.9209440000 -1.3429870000
 C 1.5452160000 1.0604650000 1.1006020000
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 C 1.5973720000 -0.8505890000 2.4549890000
 C 2.1115330000 -0.1391160000 3.5401800000
 C 2.3527340000 1.2299800000 3.3791580000
 C 2.0692190000 1.8356970000 2.1481130000
 C 3.0576920000 1.5814380000 -2.0991920000
 C 3.8362550000 0.8555720000 -3.0083490000
 C 3.6196040000 -0.5201190000 -3.1430230000

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 H 0.8790410000 3.6941750000 0.4246930000
 H 2.5513980000 3.3657480000 -0.0912070000
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 H 1.3942420000 -1.9244530000 2.5259210000
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 H 2.2604540000 2.9013370000 2.0160400000
 H 3.2236110000 2.6527970000 -1.9828400000
 H 4.6031200000 1.3648320000 -3.6003170000
 H 4.2019380000 -1.1309680000 -3.8384200000
 H 2.4203800000 -2.1822780000 -2.4291840000
 Fe 0.4314340000 -1.3768780000 -0.3002340000
 H -0.8670940000 3.4568510000 -0.9488960000
 N 1.5536280000 -2.8964380000 -0.0980340000
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 H -1.3200360000 -2.2127780000 -2.4611410000
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 H -4.0992050000 0.6115320000 -0.6679220000
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 C 3.1340060000 -4.9499100000 0.2983210000
 H 3.1015970000 -5.2351960000 1.3633560000
 H 4.1678670000 -4.6795440000 0.0247890000
 H 2.8018600000 -5.8020760000 -0.3176030000

[(bpyPy₂Me)Fe(MeCN)(NH₃)]²⁺, multiplicity = 5

C -2.5913420000 2.1732430000 -0.9514330000
 C -3.0444050000 0.8798530000 -0.6775890000
 C -2.0961820000 -0.1107950000 -0.3766080000
 N -0.7665160000 0.1721160000 -0.3849780000
 C -0.3203310000 1.4345020000 -0.5466250000
 C -1.2233960000 2.4662420000 -0.8555790000
 C -3.7585250000 -1.9490980000 0.2003710000
 C -2.4386660000 -1.4910890000 0.0435500000
 C -3.9810450000 -3.2470860000 0.6720410000
 C -2.8822570000 -4.0624810000 0.9766090000
 C -1.5965210000 -3.5496450000 0.7807710000
 N -1.3776460000 -2.2993740000 0.3275740000

C 1.1949840000 1.6837070000 -0.2930150000
 C 1.4682350000 3.2004550000 -0.2816540000
 C 2.0595490000 0.9972930000 -1.3824250000
 C 1.5627530000 1.0638920000 1.0897630000
 N 1.4487890000 -0.2801680000 1.2376680000
 C 1.7644720000 -0.8621850000 2.4147980000
 C 2.2057320000 -0.1338270000 3.5208370000
 C 2.3253150000 1.2532990000 3.3879390000
 C 2.0032010000 1.8553060000 2.1642040000
 C 2.9624920000 1.7169350000 -2.1857690000
 C 3.7566890000 1.0369030000 -3.1174860000
 C 3.6419020000 -0.3531080000 -3.2296610000
 C 2.7187840000 -1.0021370000 -2.4083180000
 N 1.9448120000 -0.3440370000 -1.5182120000
 H -3.3029320000 2.9640690000 -1.2059870000
 H -5.0029410000 -3.6156390000 0.8024300000
 H -3.0117400000 -5.0808990000 1.3517550000
 H -0.7077980000 -4.1552780000 0.9847850000
 H 0.8445620000 3.7036890000 0.4721460000
 H 2.5239650000 3.4062520000 -0.0501460000
 H 1.2406700000 3.6447870000 -1.2624190000
 H 1.6563810000 -1.9517240000 2.4612080000
 H 2.4508390000 -0.6479160000 4.4542570000
 H 2.6698910000 1.8691410000 4.2244400000
 H 2.1017700000 2.9363690000 2.0601310000
 H 3.0589270000 2.7988620000 -2.0894260000
 H 4.4622250000 1.5939950000 -3.7421260000
 H 4.2487460000 -0.9281170000 -3.9346370000
 H 2.5855770000 -2.0881270000 -2.4546760000
 Fe 0.5269130000 -1.4856610000 -0.3052620000
 H -0.8803890000 3.4885080000 -1.0158050000
 N 1.7136470000 -3.1823430000 -0.0153630000
 N -0.1855920000 -2.2733400000 -2.2998310000
 H -1.2044920000 -2.2068480000 -2.4235270000
 H 0.0396140000 -3.2663820000 -2.4431900000
 H 0.2133460000 -1.7778280000 -3.1063020000
 H -4.6034930000 -1.2982370000 -0.0356300000
 H -4.1128770000 0.6528260000 -0.6889350000
 C 2.3960080000 -4.1115610000 0.1642010000
 C 3.2508080000 -5.2641530000 0.3855240000
 H 3.2304940000 -5.5401030000 1.4528750000
 H 4.2831960000 -5.0132540000 0.0890140000
 H 2.8904250000 -6.1101210000 -0.2228040000

[(bpyPy₂Me)Fe(N₂H₄)(NH₃)]²⁺, multiplicity = 1

C -2.5311680000 2.2158950000 -0.9662520000
C -2.9964880000 0.9156060000 -0.7445590000
C -2.0568180000 -0.1008550000 -0.5200790000
N -0.7172990000 0.1572450000 -0.6052750000
C -0.2621780000 1.4298830000 -0.6511140000
C -1.1570080000 2.4881510000 -0.8622560000
C -3.6124250000 -1.9680340000 0.2236470000
C -2.3292670000 -1.4520730000 -0.0146090000
C -3.7493290000 -3.2107110000 0.8487580000
C -2.5904050000 -3.9021860000 1.2272430000
C -1.3423420000 -3.3434040000 0.9400920000
N -1.1897470000 -2.1520470000 0.3187460000
C 1.2417600000 1.5864010000 -0.3402380000
C 1.6144190000 3.0755470000 -0.2551220000
C 2.0647750000 0.8648050000 -1.4188950000
C 1.4870000000 0.8669310000 1.0147370000
N 1.1608740000 -0.4567800000 1.0937370000
C 1.2998900000 -1.1044610000 2.2780470000
C 1.8022620000 -0.4884520000 3.4225820000
C 2.1719100000 0.8595230000 3.3464670000
C 2.0036860000 1.5381890000 2.1339000000
C 3.0100580000 1.5268920000 -2.2175570000
C 3.7276760000 0.8215280000 -3.1895080000
C 3.4796980000 -0.5473370000 -3.3398880000
C 2.5307550000 -1.1467500000 -2.5149760000
N 1.8280490000 -0.4678390000 -1.5668570000
H -3.2372110000 3.0288160000 -1.1585290000
H -4.7417710000 -3.6270020000 1.0440400000
H -2.6392350000 -4.8697740000 1.7336750000
H -0.4348620000 -3.8845640000 1.2220750000
H 1.0171780000 3.5806620000 0.5192210000
H 2.6796750000 3.2025520000 -0.0099370000
H 1.4208390000 3.5757220000 -1.2163830000
H 0.9839610000 -2.1515960000 2.2975900000
H 1.8954770000 -1.0624030000 4.3483430000
H 2.5770010000 1.3827870000 4.2177290000
H 2.2740620000 2.5925370000 2.0655540000
H 3.1871020000 2.5948060000 -2.0852810000
H 4.4639720000 1.3350080000 -3.8147860000
H 4.0075670000 -1.1541090000 -4.0804360000
H 2.3184580000 -2.2146420000 -2.6166500000
Fe 0.4407880000 -1.3387660000 -0.4885150000
H -0.7989910000 3.5161960000 -0.9350340000
N 1.6166560000 -2.9986050000 -0.2531350000
H 1.6297220000 -3.5603360000 -1.1168580000
H 1.1999820000 -3.6570130000 0.4184420000

N -0.3047020000 -2.1396150000 -2.2083820000
 H -1.2775510000 -1.8419740000 -2.3691680000
 H -0.3382760000 -3.1685140000 -2.2324920000
 H 0.1944130000 -1.8579710000 -3.0626450000
 N 3.0270290000 -2.9312410000 0.1535600000
 H -4.4933830000 -1.3916630000 -0.0698180000
 H -4.0675550000 0.7013380000 -0.7121780000
 H 3.4802590000 -2.3051930000 -0.5251420000
 H 3.0343470000 -2.3935700000 1.0304540000

[(bpyPy₂Me)Fe(N₂H₄)(NH₃)]²⁺, multiplicity = 3

C -2.5298590000 2.1912600000 -0.8523600000
 C -3.0066840000 0.8996760000 -0.6233860000
 C -2.0804990000 -0.1251500000 -0.3830640000
 N -0.7313200000 0.1161450000 -0.4232790000
 C -0.2609060000 1.3867640000 -0.5298410000
 C -1.1516710000 2.4433370000 -0.7668370000
 C -3.7169530000 -1.9825640000 0.1806700000
 C -2.4096030000 -1.4949390000 0.0099410000
 C -3.9075850000 -3.2891690000 0.6342430000
 C -2.7813080000 -4.0818560000 0.9068790000
 C -1.5111300000 -3.5437220000 0.7002060000
 N -1.3100070000 -2.2800030000 0.2596710000
 C 1.2529720000 1.5980190000 -0.2919360000
 C 1.5843070000 3.1019130000 -0.3112410000
 C 2.0768780000 0.8503860000 -1.3648030000
 C 1.5822070000 0.9889940000 1.1015650000
 N 1.3151760000 -0.3287420000 1.2743010000
 C 1.5342050000 -0.9037510000 2.4792610000
 C 2.0492270000 -0.2002430000 3.5681830000
 C 2.3509610000 1.1558080000 3.3959850000
 C 2.1125180000 1.7551340000 2.1530840000
 C 3.0581160000 1.4954050000 -2.1383650000
 C 3.7682310000 0.7742820000 -3.1041670000
 C 3.4822400000 -0.5839420000 -3.2849330000
 C 2.5017780000 -1.1605060000 -2.4794220000
 N 1.8210270000 -0.4682200000 -1.5364310000
 H -3.2247980000 3.0100320000 -1.0592430000
 H -4.9180210000 -3.6837010000 0.7750890000
 H -2.8779020000 -5.1093960000 1.2673330000
 H -0.6239960000 -4.1544980000 0.8886290000
 H 0.9924130000 3.6396810000 0.4446030000
 H 2.6493890000 3.2704840000 -0.0938880000
 H 1.3635340000 3.5360210000 -1.2981850000
 H 1.2789250000 -1.9653280000 2.5714870000

H 2.2067290000 -0.7102090000 4.5223700000
 H 2.7636330000 1.7477050000 4.2187010000
 H 2.3400020000 2.8126590000 2.0144640000
 H 3.2706650000 2.5551490000 -1.9964210000
 H 4.5301870000 1.2735620000 -3.7105320000
 H 3.9995820000 -1.1896530000 -4.0336810000
 H 2.2312840000 -2.2139390000 -2.5994560000
 Fe 0.4200680000 -1.4117840000 -0.3108980000
 H -0.7841690000 3.4634630000 -0.8807960000
 N 1.5711780000 -3.0641470000 -0.0564850000
 H 1.4148000000 -3.7334140000 -0.8234460000
 H 1.2399040000 -3.5850740000 0.7690220000
 N -0.3680710000 -2.2503840000 -2.4324230000
 H -1.3960100000 -2.2373610000 -2.4274440000
 H -0.1244980000 -3.2081770000 -2.7174640000
 H -0.1022850000 -1.6560710000 -3.2277480000
 N 3.0250010000 -3.0124930000 0.1298570000
 H -4.5734120000 -1.3393790000 -0.0354300000
 H -4.0789250000 0.6905920000 -0.6169730000
 H 3.4145540000 -2.6910410000 -0.7649480000
 H 3.1922950000 -2.2297610000 0.7754710000

[(bpyPy₂Me)Fe(N₂H₄)(NH₃)]²⁺, multiplicity = 5

C -2.5482370000 2.2118170000 -0.8660130000
 C -3.0251570000 0.9251060000 -0.6068490000
 C -2.0937800000 -0.0966560000 -0.3591690000
 N -0.7586960000 0.1513340000 -0.4039240000
 C -0.2862710000 1.4083310000 -0.5442900000
 C -1.1712460000 2.4688220000 -0.8020160000
 C -3.7921790000 -1.9055510000 0.1736860000
 C -2.4601980000 -1.4741410000 0.0394540000
 C -4.0529030000 -3.2068280000 0.6129930000
 C -2.9731820000 -4.0499850000 0.9104200000
 C -1.6755960000 -3.5578620000 0.7444540000
 N -1.4126800000 -2.3038770000 0.3204060000
 C 1.2370490000 1.6227490000 -0.3098900000
 C 1.5418620000 3.1338850000 -0.2862040000
 C 2.0760530000 0.9349000000 -1.4148400000
 C 1.5931300000 0.9836710000 1.0674650000
 N 1.4073100000 -0.3533940000 1.2212580000
 C 1.6627960000 -0.9269670000 2.4190380000
 C 2.1343450000 -0.2135900000 3.5210270000
 C 2.3473130000 1.1607380000 3.3712620000
 C 2.0703260000 1.7614040000 2.1371760000
 C 3.0057340000 1.6427730000 -2.1978210000

C 3.7547200000 0.9676740000 -3.1688450000
 C 3.5619880000 -0.4064470000 -3.3480620000
 C 2.6164840000 -1.0428180000 -2.5442010000
 N 1.8973070000 -0.3934700000 -1.6018200000
 H -3.2468460000 3.0258520000 -1.0807420000
 H -5.0841530000 -3.5552030000 0.7228620000
 H -3.1250900000 -5.0739900000 1.2623210000
 H -0.8140980000 -4.1973030000 0.9602440000
 H 0.9369610000 3.6414820000 0.4801210000
 H 2.6036240000 3.3161940000 -0.0637840000
 H 1.3141980000 3.5911340000 -1.2606860000
 H 1.4742620000 -2.0026150000 2.4962500000
 H 2.3259980000 -0.7301550000 4.4653740000
 H 2.7203890000 1.7664250000 4.2028610000
 H 2.2276420000 2.8337620000 2.0203790000
 H 3.1531670000 2.7138750000 -2.0595630000
 H 4.4787800000 1.5166420000 -3.7789390000
 H 4.1206670000 -0.9770260000 -4.0947370000
 H 2.4141170000 -2.1127150000 -2.6601430000
 Fe 0.5180970000 -1.5432720000 -0.3760180000
 H -0.8077010000 3.4867210000 -0.9444220000
 N 1.6235250000 -3.3676580000 0.1303610000
 H 1.4332610000 -4.1268230000 -0.5379230000
 H 1.3588850000 -3.7869510000 1.0330130000
 N -0.2361700000 -2.3391660000 -2.3441890000
 H -1.2551340000 -2.4759060000 -2.3357210000
 H 0.1462760000 -3.2416450000 -2.6558170000
 H -0.0626590000 -1.6893870000 -3.1218820000
 N 3.0897250000 -3.2460880000 0.1873860000
 H -4.6181890000 -1.2297160000 -0.0592890000
 H -4.0988540000 0.7264980000 -0.5854740000
 H 3.4028070000 -3.1885520000 -0.7894640000
 H 3.2746050000 -2.3081820000 0.5684080000

[(bpyPy₂Me)Fe(NH₃)(N₂H₄)]²⁺, multiplicity = 1

C -2.5696540000 2.2279200000 -0.9630660000
 C -3.0387160000 0.9305160000 -0.7306690000
 C -2.1017520000 -0.0874850000 -0.5034830000
 N -0.7603950000 0.1663290000 -0.5928590000
 C -0.3006750000 1.4382070000 -0.6474420000
 C -1.1939210000 2.4963110000 -0.8653060000
 C -3.6556790000 -1.9607600000 0.2383530000
 C -2.3743910000 -1.4379400000 0.0025820000
 C -3.7860230000 -3.2086950000 0.8541720000
 C -2.6238600000 -3.9012930000 1.2237960000

C -1.3772960000 -3.3364040000 0.9432160000
N -1.2328610000 -2.1358700000 0.3347230000
C 1.2027660000 1.5977860000 -0.3318120000
C 1.5771190000 3.0874310000 -0.2687210000
C 2.0411260000 0.8570700000 -1.3866440000
C 1.4473470000 0.8962550000 1.0327290000
N 1.1184090000 -0.4253320000 1.1286250000
C 1.2860800000 -1.0671130000 2.3110180000
C 1.8128250000 -0.4433150000 3.4401910000
C 2.1759030000 0.9051740000 3.3499010000
C 1.9836790000 1.5765350000 2.1367720000
C 3.0084560000 1.4956610000 -2.1771270000
C 3.7407630000 0.7623130000 -3.1181730000
C 3.4843440000 -0.6071860000 -3.2473370000
C 2.5144210000 -1.1849930000 -2.4303860000
N 1.8006080000 -0.4764370000 -1.5126390000
H -3.2731420000 3.0420650000 -1.1592980000
H -4.7764590000 -3.6303230000 1.0473900000
H -2.6707600000 -4.8757900000 1.7160910000
H -0.4621090000 -3.8712430000 1.2078690000
H 0.9790160000 3.6064470000 0.4952870000
H 2.6414900000 3.2159840000 -0.0208490000
H 1.3892420000 3.5726500000 -1.2389650000
H 0.9761020000 -2.1144020000 2.3436670000
H 1.9300090000 -1.0124900000 4.3664030000
H 2.5974760000 1.4336630000 4.2101790000
H 2.2541600000 2.6299580000 2.0559040000
H 3.1923810000 2.5645270000 -2.0620330000
H 4.4952160000 1.2571450000 -3.7371520000
H 4.0221650000 -1.2308980000 -3.9667150000
H 2.2838070000 -2.2516190000 -2.5147350000
Fe 0.3926610000 -1.3226100000 -0.4454510000
H -0.8333400000 3.5225360000 -0.9477020000
N 1.5915010000 -2.9308940000 -0.1704920000
H 1.4552400000 -3.5640590000 -0.9794200000
H 1.4311660000 -3.4992860000 0.6701150000
N -0.2989200000 -2.1300320000 -2.1934380000
H -1.3101790000 -1.9466580000 -2.3139330000
N -0.0044360000 -3.5345430000 -2.4131440000
H 0.1473620000 -1.6185990000 -2.9660150000
H 2.5890590000 -2.6844270000 -0.1375390000
H -4.5391010000 -1.3867940000 -0.0521210000
H -4.1104260000 0.7191150000 -0.6938030000
H -0.2897230000 -3.7787080000 -3.3709880000
H -0.6362040000 -4.0640930000 -1.7991960000

[(bpyPy₂Me)Fe(NH₃)(N₂H₄)]²⁺, multiplicity = 3

C -2.5712720000 2.2311610000 -0.8495330000
C -3.0551430000 0.9422950000 -0.6183810000
C -2.1353190000 -0.0843620000 -0.3638540000
N -0.7837850000 0.1530830000 -0.3917340000
C -0.3069380000 1.4207740000 -0.5061150000
C -1.1925780000 2.4787270000 -0.7557830000
C -3.7723720000 -1.9391780000 0.2178720000
C -2.4670140000 -1.4500610000 0.0384540000
C -3.9570200000 -3.2376290000 0.6970290000
C -2.8276310000 -4.0188290000 0.9918100000
C -1.5580460000 -3.4819360000 0.7756640000
N -1.3653430000 -2.2281880000 0.3000650000
C 1.2079730000 1.6239970000 -0.2734060000
C 1.5480950000 3.1257180000 -0.2982500000
C 2.0289690000 0.8647090000 -1.3416670000
C 1.5571610000 1.0129210000 1.1149900000
N 1.3006570000 -0.3064150000 1.2829550000
C 1.5792950000 -0.9021990000 2.4638490000
C 2.1304480000 -0.2091950000 3.5420190000
C 2.4060170000 1.1540450000 3.3813490000
C 2.1178320000 1.7702310000 2.1569930000
C 3.0161830000 1.4995800000 -2.1147870000
C 3.7461590000 0.7627410000 -3.0540450000
C 3.4766760000 -0.6018560000 -3.2038930000
C 2.4862100000 -1.1695870000 -2.4035350000
N 1.7780810000 -0.4584260000 -1.4938750000
H -3.2613050000 3.0514810000 -1.0664880000
H -4.9658300000 -3.6337940000 0.8450830000
H -2.9223880000 -5.0367720000 1.3791980000
H -0.6638980000 -4.0741550000 0.9879130000
H 0.9633100000 3.6681230000 0.4599910000
H 2.6151700000 3.2885730000 -0.0867750000
H 1.3251960000 3.5595620000 -1.2848370000
H 1.3453370000 -1.9693700000 2.5404670000
H 2.3363100000 -0.7322730000 4.4799060000
H 2.8422200000 1.7377850000 4.1978390000
H 2.3332240000 2.8312240000 2.0249900000
H 3.2200550000 2.5633570000 -1.9914360000
H 4.5133930000 1.2543570000 -3.6600480000
H 4.0146300000 -1.2221780000 -3.9257730000
H 2.2383510000 -2.2314130000 -2.4991460000
Fe 0.3542790000 -1.3706890000 -0.2665630000
H -0.8204110000 3.4965620000 -0.8747360000
N 1.5049420000 -3.0173240000 -0.1549970000
H 1.3031600000 -3.5760850000 -1.0131690000

H 1.3447640000 -3.6417900000 0.6459360000
N -0.3911300000 -2.3049290000 -2.4043630000
H -1.3917340000 -2.1969740000 -2.6312710000
N 0.0232850000 -3.6874690000 -2.5236300000
H 0.1057810000 -1.7807910000 -3.1332710000
H 2.5137850000 -2.8197630000 -0.1463560000
H -4.6313770000 -1.3027420000 -0.0085130000
H -4.1280970000 0.7363070000 -0.6214140000
H -0.1510470000 -4.0259830000 -3.4806430000
H -0.6153990000 -4.2336520000 -1.9317550000

[(bpyPy₂Me)Fe(NH₃)(N₂H₄)]²⁺, multiplicity = 5

C -2.5819470000 2.2386670000 -0.8673160000
C -3.0693090000 0.9558290000 -0.6081790000
C -2.1474640000 -0.0699330000 -0.3417270000
N -0.8088790000 0.1701430000 -0.3713090000
C -0.3269520000 1.4230430000 -0.5202120000
C -1.2034190000 2.4868780000 -0.7913920000
C -3.8604330000 -1.8630410000 0.2127120000
C -2.5266230000 -1.4409890000 0.0666120000
C -4.1261150000 -3.1542310000 0.6774160000
C -3.0512170000 -3.9999590000 0.9883710000
C -1.7512080000 -3.5216620000 0.8064900000
N -1.4857350000 -2.2770440000 0.3554630000
C 1.1983720000 1.6263530000 -0.2908030000
C 1.5196040000 3.1337480000 -0.2888440000
C 2.0273340000 0.9103600000 -1.3882340000
C 1.5667800000 1.0000010000 1.0888120000
N 1.3861470000 -0.3348450000 1.2487410000
C 1.6957780000 -0.9214560000 2.4256860000
C 2.2023560000 -0.2103110000 3.5140120000
C 2.3924720000 1.1679190000 3.3667560000
C 2.0721170000 1.7762260000 2.1462650000
C 2.9701040000 1.5925140000 -2.1783340000
C 3.7202390000 0.8883190000 -3.1282890000
C 3.5186060000 -0.4881990000 -3.2758890000
C 2.5609930000 -1.0998360000 -2.4655490000
N 1.8351260000 -0.4192890000 -1.5499940000
H -3.2727320000 3.0560610000 -1.0936500000
H -5.1589520000 -3.4937980000 0.7993370000
H -3.2104580000 -5.0146870000 1.3621600000
H -0.8879770000 -4.1562580000 1.0310080000
H 0.9252180000 3.6582040000 0.4738160000
H 2.5844370000 3.3078220000 -0.0737960000
H 1.2915060000 3.5819270000 -1.2678520000

H 1.5253770000 -2.0019580000 2.4897190000
 H 2.4400010000 -0.7299210000 4.4462820000
 H 2.7883700000 1.7707180000 4.1899150000
 H 2.2232970000 2.8499130000 2.0305490000
 H 3.1298240000 2.6644410000 -2.0594750000
 H 4.4553370000 1.4171260000 -3.7431950000
 H 4.0818660000 -1.0807480000 -4.0019940000
 H 2.3523510000 -2.1728490000 -2.5528160000
 Fe 0.4356390000 -1.5296630000 -0.2829110000
 H -0.8324730000 3.5012390000 -0.9384000000
 N 1.6528660000 -3.2930540000 -0.0127230000
 H 1.5604010000 -3.8277970000 -0.8944180000
 H 1.4552520000 -3.9514370000 0.7517580000
 N -0.2934890000 -2.3494780000 -2.2995610000
 H -1.3086030000 -2.2749180000 -2.4738960000
 N 0.1795150000 -3.6992450000 -2.5499660000
 H 0.1378580000 -1.7496330000 -3.0127190000
 H 2.6492460000 -3.0584770000 0.0846210000
 H -4.6840450000 -1.1869490000 -0.0282010000
 H -4.1447320000 0.7634940000 -0.6007900000
 H -0.0806740000 -3.9727370000 -3.5081250000
 H -0.3790740000 -4.3152390000 -1.9456070000

[(bpyPy₂Me)Fe(η^2 -N₂H₄)]²⁺, multiplicity = 1

C -2.6032110000 2.4256830000 -0.9365670000
 C -3.1273900000 1.1389800000 -0.7644410000
 C -2.2365520000 0.0745180000 -0.5796810000
 N -0.8841760000 0.2730210000 -0.6621170000
 C -0.3734000000 1.5243730000 -0.6500170000
 C -1.2192780000 2.6303800000 -0.8189780000
 C -3.8547750000 -1.7642010000 0.1249580000
 C -2.5618790000 -1.2757110000 -0.1119160000
 C -4.0153150000 -3.0127850000 0.7353950000
 C -2.8737180000 -3.7344660000 1.1110170000
 C -1.6118100000 -3.2043230000 0.8262430000
 N -1.4438250000 -2.0132640000 0.2063350000
 C 1.1340540000 1.5948170000 -0.3448110000
 C 1.5693500000 3.0587770000 -0.1672330000
 C 1.9059600000 0.9083120000 -1.4836150000
 C 1.4061110000 0.7720130000 0.9449820000
 N 1.0541110000 -0.5462160000 0.9356220000
 C 1.3095230000 -1.3180620000 2.0211610000
 C 1.9218520000 -0.8180820000 3.1680940000
 C 2.2805970000 0.5351430000 3.1984110000
 C 2.0205030000 1.3308250000 2.0764990000

C 2.8682180000 1.5911080000 -2.2432100000
 C 3.5624210000 0.9313460000 -3.2615390000
 C 3.2739150000 -0.4170000000 -3.4902040000
 C 2.3067170000 -1.0353660000 -2.7016520000
 N 1.6157040000 -0.4052360000 -1.7150510000
 H -3.2715150000 3.2764970000 -1.0968520000
 H -5.0166060000 -3.4097660000 0.9257520000
 H -2.9473830000 -4.7024680000 1.6135890000
 H -0.7051680000 -3.7510400000 1.1038190000
 H 1.0059240000 3.5286660000 0.6534650000
 H 2.6427310000 3.1279620000 0.0642720000
 H 1.3782350000 3.6327470000 -1.0866140000
 H 1.0098200000 -2.3666760000 1.9480010000
 H 2.1076510000 -1.4836400000 4.0153640000
 H 2.7597400000 0.9701970000 4.0806280000
 H 2.2994790000 2.3850760000 2.0869280000
 H 3.0778090000 2.6416660000 -2.0401780000
 H 4.3119870000 1.4611920000 -3.8566020000
 H 3.7830250000 -0.9974520000 -4.2641490000
 H 2.0946130000 -2.0899760000 -2.8878160000
 Fe 0.1855120000 -1.2727160000 -0.6272230000
 H -0.8138000000 3.6430400000 -0.8454590000
 N -0.1763700000 -2.5830510000 -2.0687110000
 H -1.0278420000 -3.1592010000 -2.1038070000
 N 0.7755820000 -3.1057860000 -1.1160200000
 H 0.2102290000 -2.5261080000 -3.0211370000
 H -4.7240960000 -1.1650970000 -0.1577710000
 H -4.2069650000 0.9711520000 -0.7368650000
 H 1.6788060000 -3.3364830000 -1.5522330000
 H 0.4244720000 -3.9646270000 -0.6725540000

[(bpyPy₂Me)Fe(η^2 -N₂H₄)]²⁺, multiplicity = 3 (N₂H₄ becomes η^2)

C -2.5596350000 2.6162900000 -0.4511670000
 C -3.1367980000 1.3449530000 -0.4503820000
 C -2.2967180000 0.2249830000 -0.3991480000
 N -0.9338270000 0.3607690000 -0.3776680000
 C -0.3638640000 1.5906890000 -0.3416820000
 C -1.1649290000 2.7411720000 -0.3805410000
 C -4.0687780000 -1.5895320000 -0.2504110000
 C -2.7317180000 -1.1658710000 -0.3025400000
 C -4.3519250000 -2.9450540000 -0.0682810000
 C -3.2854290000 -3.8471990000 0.0709060000
 C -1.9788320000 -3.3675230000 -0.0057210000
 N -1.6898220000 -2.0570340000 -0.2078840000
 C 1.1751790000 1.6273540000 -0.2522360000

C 1.6751850000 3.0815150000 -0.1795900000
 C 1.7286440000 0.9251590000 -1.5167770000
 C 1.5948290000 0.8472120000 1.0234280000
 N 1.1549760000 -0.4304950000 1.1445880000
 C 1.4466940000 -1.1474010000 2.2554360000
 C 2.2048610000 -0.6262550000 3.3028040000
 C 2.6864340000 0.6826100000 3.1831090000
 C 2.3783440000 1.4241510000 2.0359310000
 C 2.6196890000 1.5566430000 -2.3979510000
 C 3.0414810000 0.8908930000 -3.5556000000
 C 2.5692050000 -0.4007840000 -3.8107420000
 C 1.7029690000 -0.9860640000 -2.8874630000
 N 1.2959170000 -0.3371760000 -1.7684580000
 H -3.1886520000 3.5098980000 -0.4926130000
 H -5.3881260000 -3.2922150000 -0.0239940000
 H -3.4553710000 -4.9143600000 0.2358090000
 H -1.1350920000 -4.0527350000 0.1063490000
 H 1.2606480000 3.5895410000 0.7041540000
 H 2.7726440000 3.1146210000 -0.1108430000
 H 1.3709590000 3.6417530000 -1.0764430000
 H 1.0498600000 -2.1671020000 2.2996700000
 H 2.4103670000 -1.2389880000 4.1845330000
 H 3.2950580000 1.1298590000 3.9749560000
 H 2.7496710000 2.4448880000 1.9398260000
 H 2.9867090000 2.5623150000 -2.1916810000
 H 3.7328370000 1.3829750000 -4.2466580000
 H 2.8668000000 -0.9579610000 -4.7031620000
 H 1.3320100000 -2.0122340000 -3.0018980000
 Fe 0.1051230000 -1.2516060000 -0.4022010000
 H -0.7115440000 3.7324590000 -0.3569150000
 N 0.9049120000 -3.7447820000 -1.6949400000
 H -0.0798020000 -4.0342440000 -1.6790630000
 N 1.1471220000 -2.9686490000 -0.4932190000
 H 1.4565250000 -4.6113370000 -1.6349320000
 H -4.8764690000 -0.8594730000 -0.3421750000
 H -4.2217630000 1.2210450000 -0.4788470000
 H 2.1466580000 -2.7223890000 -0.5102050000
 H 1.0363600000 -3.5465940000 0.3580470000

[(bpyPy₂Me)Fe(η^2 -N₂H₄)]²⁺, multiplicity = 5 (N₂H₄ becomes η^2)

C -2.5765780000 2.6266260000 -0.4069460000
 C -3.1518020000 1.3532670000 -0.3886770000
 C -2.3025170000 0.2379480000 -0.3297150000
 N -0.9544830000 0.3866960000 -0.3016940000
 C -0.3838380000 1.6077310000 -0.3029860000

C -1.1827760000 2.7625400000 -0.3565830000
 C -4.1245000000 -1.5274930000 -0.2360700000
 C -2.7682280000 -1.1642260000 -0.2672100000
 C -4.4735580000 -2.8779690000 -0.1365400000
 C -3.4570970000 -3.8395920000 -0.0639930000
 C -2.1287810000 -3.4103470000 -0.1064440000
 N -1.7837500000 -2.1087820000 -0.2132400000
 C 1.1682790000 1.6505290000 -0.2395530000
 C 1.6467040000 3.1146080000 -0.1948100000
 C 1.7294770000 0.9482010000 -1.5084390000
 C 1.6338400000 0.9025520000 1.0440770000
 N 1.3196480000 -0.4130680000 1.1728090000
 C 1.6841950000 -1.1007340000 2.2795030000
 C 2.3841650000 -0.5092590000 3.3302600000
 C 2.7238050000 0.8428770000 3.2141080000
 C 2.3477350000 1.5510310000 2.0655600000
 C 2.5366610000 1.6228020000 -2.4385940000
 C 3.0002770000 0.9498100000 -3.5766390000
 C 2.6557200000 -0.3918280000 -3.7689280000
 C 1.8582150000 -1.0130520000 -2.8071570000
 N 1.4070800000 -0.3548530000 -1.7125920000
 H -3.2109300000 3.5164970000 -0.4541230000
 H -5.5266260000 -3.1730700000 -0.1104300000
 H -3.6796450000 -4.9061940000 0.0237370000
 H -1.3119920000 -4.1352800000 -0.0501120000
 H 1.2335360000 3.6313080000 0.6842510000
 H 2.7444640000 3.1656990000 -0.1421890000
 H 1.3199580000 3.6573580000 -1.0941250000
 H 1.3984290000 -2.1575060000 2.3138110000
 H 2.6562380000 -1.1008790000 4.2082860000
 H 3.2793930000 1.3505820000 4.0085970000
 H 2.6140670000 2.6043630000 1.9780600000
 H 2.8091820000 2.6672830000 -2.2876880000
 H 3.6293860000 1.4764810000 -4.3009900000
 H 2.9987760000 -0.9566210000 -4.6399820000
 H 1.5741600000 -2.0721660000 -2.8790320000
 Fe 0.2139010000 -1.3658240000 -0.3137820000
 H -0.7378260000 3.7578180000 -0.3592410000
 N 0.9818440000 -3.9534090000 -1.7501540000
 H -0.0257070000 -4.0932590000 -1.8896410000
 N 1.1494280000 -3.3085690000 -0.4597670000
 H 1.3897450000 -4.8967570000 -1.7020440000
 H -4.9014280000 -0.7612870000 -0.2834930000
 H -4.2370720000 1.2347460000 -0.4166160000
 H 2.1533180000 -3.0969330000 -0.3744540000
 H 0.9570860000 -3.9617010000 0.3171290000

[(bpyPy₂Me)Fe(NH₃)(NH₃)]²⁺, multiplicity = 1

C -2.5605910000 2.2304990000 -0.9564740000
C -3.0243190000 0.9305810000 -0.7271440000
C -2.0832920000 -0.0853100000 -0.5077570000
N -0.7433390000 0.1745760000 -0.6010550000
C -0.2882560000 1.4476180000 -0.6506570000
C -1.1856630000 2.5036500000 -0.8619830000
C -3.6281480000 -1.9728010000 0.2220590000
C -2.3504910000 -1.4412330000 -0.0119890000
C -3.7489310000 -3.2313500000 0.8187950000
C -2.5820980000 -3.9258120000 1.1686050000
C -1.3391320000 -3.3514810000 0.8899890000
N -1.2057150000 -2.1390110000 0.3050230000
C 1.2146090000 1.6095200000 -0.3341580000
C 1.5829600000 3.1002130000 -0.2599530000
C 2.0590820000 0.8790610000 -1.3905290000
C 1.4551340000 0.8999370000 1.0272220000
N 1.1251670000 -0.4226930000 1.1164660000
C 1.2672930000 -1.0598360000 2.3045790000
C 1.7784770000 -0.4375240000 3.4416910000
C 2.1519790000 0.9080970000 3.3546970000
C 1.9788360000 1.5785350000 2.1382620000
C 3.0296610000 1.5279520000 -2.1687870000
C 3.7764780000 0.8045970000 -3.1060080000
C 3.5320400000 -0.5662340000 -3.2413560000
C 2.5561310000 -1.1522360000 -2.4375050000
N 1.8252150000 -0.4547180000 -1.5258500000
H -3.2676520000 3.0426550000 -1.1480380000
H -4.7364240000 -3.6603230000 1.0110820000
H -2.6224710000 -4.9089670000 1.6440060000
H -0.4195110000 -3.8877750000 1.1364890000
H 0.9800640000 3.6119840000 0.5051220000
H 2.6458700000 3.2316970000 -0.0076150000
H 1.3962150000 3.5906420000 -1.2277830000
H 0.9454570000 -2.1040180000 2.3408990000
H 1.8745750000 -1.0054940000 4.3710510000
H 2.5634290000 1.4359050000 4.2202300000
H 2.2523700000 2.6313930000 2.0607840000
H 3.2059310000 2.5972040000 -2.0458950000
H 4.5338760000 1.3072230000 -3.7149800000
H 4.0835870000 -1.1849920000 -3.9546090000
H 2.3423190000 -2.2204590000 -2.5262350000
Fe 0.4112640000 -1.3127480000 -0.4728970000
H -0.8288220000 3.5313600000 -0.9422450000

N 1.5938680000 -2.9432600000 -0.1827150000
 H 1.3335010000 -3.7789830000 -0.7233570000
 H 1.6287350000 -3.2633740000 0.7940230000
 N -0.2921230000 -2.1139980000 -2.2082680000
 H -1.2854990000 -1.8878050000 -2.3613920000
 H -0.2427590000 -3.1406630000 -2.2664040000
 H 0.1867800000 -1.7606280000 -3.0467610000
 H 2.5798910000 -2.7637880000 -0.4178540000
 H -4.5158600000 -1.3990850000 -0.0555210000
 H -4.0951250000 0.7151480000 -0.6875390000

[(bpyPy₂Me)Fe(NH₃)(NH₃)]²⁺, multiplicity = 3

C -2.5665730000 2.2053190000 -0.8308930000
 C -3.0405530000 0.9112750000 -0.6103240000
 C -2.1113650000 -0.1131910000 -0.3810760000
 N -0.7621890000 0.1323050000 -0.4247150000
 C -0.2933920000 1.4040580000 -0.5250320000
 C -1.1882940000 2.4599400000 -0.7492390000
 C -3.7318990000 -1.9930870000 0.1669680000
 C -2.4310750000 -1.4872500000 0.0021660000
 C -3.9047040000 -3.3053860000 0.6116540000
 C -2.7682570000 -4.0848450000 0.8822770000
 C -1.5037450000 -3.5309580000 0.6825080000
 N -1.3221930000 -2.2607400000 0.2491540000
 C 1.2207390000 1.6179420000 -0.2899590000
 C 1.5515450000 3.1214790000 -0.3247460000
 C 2.0579960000 0.8556710000 -1.3419770000
 C 1.5577290000 1.0204220000 1.1074960000
 N 1.2913410000 -0.2949240000 1.2881550000
 C 1.5425340000 -0.8702000000 2.4842200000
 C 2.0844460000 -0.1663160000 3.5604080000
 C 2.3772720000 1.1909070000 3.3824130000
 C 2.1098140000 1.7902200000 2.1452360000
 C 3.0352350000 1.4941910000 -2.1248570000
 C 3.7809000000 0.7541070000 -3.0490930000
 C 3.5357930000 -0.6175170000 -3.1761590000
 C 2.5515940000 -1.1873190000 -2.3700510000
 N 1.8320210000 -0.4742940000 -1.4719610000
 H -3.2637300000 3.0244290000 -1.0288090000
 H -4.9097430000 -3.7151990000 0.7474590000
 H -2.8536420000 -5.1155160000 1.2367950000
 H -0.6055280000 -4.1247300000 0.8688850000
 H 0.9646280000 3.6654640000 0.4305510000
 H 2.6178740000 3.2919210000 -0.1153270000
 H 1.3238940000 3.5473340000 -1.3138200000

H 1.2915620000 -1.9317830000 2.5819560000
 H 2.2684690000 -0.6762660000 4.5099970000
 H 2.8074400000 1.7834120000 4.1957990000
 H 2.3335540000 2.8477950000 2.0002790000
 H 3.2185540000 2.5637660000 -2.0212590000
 H 4.5403090000 1.2489120000 -3.6623480000
 H 4.0864240000 -1.2404320000 -3.8861500000
 H 2.3151010000 -2.2515960000 -2.4503720000
 Fe 0.3823190000 -1.3917140000 -0.3140810000
 H -0.8237890000 3.4818330000 -0.8564450000
 N 1.5479250000 -3.0334640000 -0.0762520000
 H 1.3168750000 -3.8047180000 -0.7168920000
 H 1.4895000000 -3.4437640000 0.8665300000
 N -0.3761560000 -2.1779020000 -2.4599190000
 H -1.4035020000 -2.1821780000 -2.4975740000
 H -0.1003600000 -3.1331570000 -2.7218550000
 H -0.0845040000 -1.5835550000 -3.2458620000
 H 2.5503190000 -2.8453790000 -0.2119970000
 H -4.5963880000 -1.3600500000 -0.0474960000
 H -4.1122600000 0.6992150000 -0.6017360000

[(bpyPy₂Me)Fe(NH₃)(NH₃)]²⁺, multiplicity = 5

C -2.5715020000 2.2063130000 -0.8765320000
 C -3.0462050000 0.9181580000 -0.6210170000
 C -2.1135290000 -0.1002490000 -0.3634260000
 N -0.7782320000 0.1535790000 -0.3963280000
 C -0.3085500000 1.4111740000 -0.5386770000
 C -1.1955250000 2.4681550000 -0.8031660000
 C -3.8073840000 -1.9192760000 0.1637910000
 C -2.4777020000 -1.4794820000 0.0322250000
 C -4.0596670000 -3.2223030000 0.6027760000
 C -2.9755840000 -4.0598730000 0.9035130000
 C -1.6804090000 -3.5617730000 0.7392510000
 N -1.4278980000 -2.3059250000 0.3142300000
 C 1.2136040000 1.6278290000 -0.3041290000
 C 1.5192800000 3.1385850000 -0.2891210000
 C 2.0588570000 0.9299960000 -1.3998280000
 C 1.5779300000 0.9941500000 1.0740550000
 N 1.3971610000 -0.3421540000 1.2300930000
 C 1.6911310000 -0.9234150000 2.4138560000
 C 2.1851100000 -0.2116130000 3.5075240000
 C 2.3802830000 1.1657560000 3.3609050000
 C 2.0728690000 1.7712850000 2.1360820000
 C 2.9855310000 1.6315350000 -2.1920430000
 C 3.7591640000 0.9400360000 -3.1321150000

C 3.5971370000 -0.4430710000 -3.2681520000
 C 2.6482490000 -1.0717450000 -2.4613840000
 N 1.8999910000 -0.4041940000 -1.5561500000
 H -3.2711020000 3.0177640000 -1.0977180000
 H -5.0889310000 -3.5773430000 0.7101680000
 H -3.1240230000 -5.0845390000 1.2550970000
 H -0.8100430000 -4.1904080000 0.9528650000
 H 0.9174640000 3.6501860000 0.4770580000
 H 2.5820390000 3.3214000000 -0.0714520000
 H 1.2885680000 3.5915900000 -1.2649500000
 H 1.5169270000 -2.0019340000 2.4844770000
 H 2.4071120000 -0.7311630000 4.4436580000
 H 2.7669000000 1.7699800000 4.1874570000
 H 2.2227160000 2.8449150000 2.0202650000
 H 3.1140120000 2.7085740000 -2.0830810000
 H 4.4823870000 1.4828520000 -3.7487710000
 H 4.1827080000 -1.0262700000 -3.9839730000
 H 2.4707040000 -2.1497890000 -2.5392450000
 Fe 0.4878270000 -1.5418700000 -0.3461820000
 H -0.8342210000 3.4868870000 -0.9455430000
 N 1.6672160000 -3.3234890000 0.0366680000
 H 1.4604420000 -4.1079410000 -0.5955050000
 H 1.6036710000 -3.7207190000 0.9836180000
 N -0.2979630000 -2.2658960000 -2.3391490000
 H -1.3215760000 -2.1908300000 -2.4038780000
 H -0.0921220000 -3.2509190000 -2.5523630000
 H 0.0585790000 -1.7346160000 -3.1434140000
 H 2.6684760000 -3.1253440000 -0.0950730000
 H -4.6374810000 -1.2487350000 -0.0703160000
 H -4.1193030000 0.7151220000 -0.6103440000

[(bpyPy₂Me)Fe(NH₂)(NH₃)]²⁺, multiplicity = 2

C -2.5866610000 2.2410720000 -0.9393080000
 C -3.0604590000 0.9461500000 -0.6999430000
 C -2.1233790000 -0.0712290000 -0.4763760000
 N -0.7886810000 0.1869430000 -0.5573040000
 C -0.3222320000 1.4472890000 -0.6367280000
 C -1.2115570000 2.5094810000 -0.8601030000
 C -3.6793800000 -1.9571610000 0.2417580000
 C -2.4012080000 -1.4342840000 -0.0010500000
 C -3.7990520000 -3.2293930000 0.8112560000
 C -2.6344620000 -3.9416990000 1.1273510000
 C -1.3890910000 -3.3738320000 0.8417460000
 N -1.2663880000 -2.1502710000 0.2837550000
 C 1.1826540000 1.6026970000 -0.3320610000

C 1.5568070000 3.0923720000 -0.2615780000
 C 2.0304920000 0.8664140000 -1.3852610000
 C 1.4383790000 0.8906990000 1.0283630000
 N 1.1356470000 -0.4348410000 1.1173860000
 C 1.3357740000 -1.0960630000 2.2819680000
 C 1.8578660000 -0.4721970000 3.4143640000
 C 2.1838930000 0.8856980000 3.3382730000
 C 1.9700840000 1.5691590000 2.1350290000
 C 2.9868990000 1.5183350000 -2.1797990000
 C 3.7668680000 0.7808730000 -3.0769890000
 C 3.5864940000 -0.6051650000 -3.1478700000
 C 2.6209400000 -1.1935260000 -2.3337870000
 N 1.8450550000 -0.4737190000 -1.4836710000
 H -3.2903890000 3.0555960000 -1.1333100000
 H -4.7870760000 -3.6534400000 1.0114220000
 H -2.6779790000 -4.9327350000 1.5857580000
 H -0.4535790000 -3.8979090000 1.0538360000
 H 0.9604600000 3.6057800000 0.5074170000
 H 2.6218930000 3.2190150000 -0.0165730000
 H 1.3652020000 3.5834330000 -1.2279080000
 H 1.0709740000 -2.1563260000 2.2781150000
 H 2.0035640000 -1.0503940000 4.3308000000
 H 2.5997170000 1.4134970000 4.2017880000
 H 2.2210610000 2.6279940000 2.0646910000
 H 3.1275080000 2.5967020000 -2.0981130000
 H 4.5112240000 1.2852690000 -3.7006490000
 H 4.1828820000 -1.2321920000 -3.8162530000
 H 2.4552400000 -2.2740980000 -2.3308700000
 Fe 0.4003340000 -1.3606740000 -0.4579400000
 H -0.8496150000 3.5334000000 -0.9584970000
 N 1.4033200000 -2.8583810000 -0.1596780000
 H 1.1872010000 -3.7993390000 -0.5086290000
 H 2.3645020000 -2.8353040000 0.1989430000
 N -0.3064670000 -2.1257460000 -2.1981600000
 H -1.1755260000 -1.6773560000 -2.5190240000
 H -0.5158670000 -3.1300910000 -2.1325900000
 H 0.3523700000 -2.0265350000 -2.9816170000
 H -4.5667990000 -1.3694870000 -0.0050720000
 H -4.1323920000 0.7382690000 -0.6607490000

[(bpyPy₂Me)Fe(NH₂)(NH₃)]²⁺, multiplicity = 4

C -2.5608920000 2.1769040000 -0.9764550000
 C -3.0538030000 0.9007430000 -0.6905690000
 C -2.1418430000 -0.1203830000 -0.3962420000
 N -0.7964660000 0.1147630000 -0.4256000000

C -0.3115440000 1.3687390000 -0.5720720000
C -1.1866020000 2.4241590000 -0.8822760000
C -3.8460600000 -1.9421020000 0.1423640000
C -2.5240650000 -1.4783290000 0.0485330000
C -4.0743870000 -3.2324940000 0.6367610000
C -2.9844950000 -4.0255830000 1.0209980000
C -1.6933160000 -3.5017030000 0.8848590000
N -1.4750680000 -2.2606540000 0.4160000000
C 1.1982740000 1.5896850000 -0.2994130000
C 1.4971260000 3.0995050000 -0.2302470000
C 2.0566000000 0.9263160000 -1.4038210000
C 1.5506790000 0.9084450000 1.0569990000
N 1.2986230000 -0.4211470000 1.2015830000
C 1.5781080000 -1.0510730000 2.3662670000
C 2.1344320000 -0.3852070000 3.4579490000
C 2.4182600000 0.9771670000 3.3257420000
C 2.1251060000 1.6248090000 2.1183810000
C 2.9831870000 1.6381980000 -2.1846840000
C 3.7628490000 0.9472750000 -3.1206520000
C 3.6154690000 -0.4390170000 -3.2450700000
C 2.6734430000 -1.0763460000 -2.4356550000
N 1.9031800000 -0.4042370000 -1.5555370000
H -3.2475370000 2.9901020000 -1.2284110000
H -5.0966750000 -3.6137150000 0.7182470000
H -3.1247650000 -5.0363850000 1.4135990000
H -0.7998940000 -4.0792890000 1.1448500000
H 0.8906120000 3.5825240000 0.5508760000
H 2.5593520000 3.2753090000 -0.0055160000
H 1.2726450000 3.5824690000 -1.1927710000
H 1.3424480000 -2.1187650000 2.4043990000
H 2.3399530000 -0.9329870000 4.3812940000
H 2.8634900000 1.5403270000 4.1515540000
H 2.3461510000 2.6870770000 2.0143190000
H 3.1067230000 2.7156090000 -2.0698410000
H 4.4861250000 1.4909420000 -3.7364100000
H 4.2163900000 -1.0211820000 -3.9490680000
H 2.5324340000 -2.1615170000 -2.4745670000
Fe 0.4178050000 -1.4587330000 -0.2914660000
H -0.8080790000 3.4343000000 -1.0383610000
N 1.4345920000 -2.9436960000 -0.0205750000
H 1.4191700000 -3.7619780000 -0.6393250000
H 2.3145700000 -2.9251000000 0.5076220000
N -0.2731640000 -2.2850580000 -2.1120950000
H -1.0933430000 -1.7929410000 -2.4895020000
H -0.5518710000 -3.2696940000 -2.0130100000
H 0.4256300000 -2.2688430000 -2.8648860000

H -4.6840300000 -1.3113760000 -0.1637270000
H -4.1284630000 0.7069190000 -0.6788060000

[(bpyPy₂Me)Fe(NH₂)(NH₃)]²⁺, multiplicity = 6

C -2.5632960000 2.1674540000 -0.9918460000
C -3.0512850000 0.8899760000 -0.6981140000
C -2.1278490000 -0.1141810000 -0.3714000000
N -0.7964970000 0.1426150000 -0.3682480000
C -0.3166620000 1.3852400000 -0.5522580000
C -1.1914110000 2.4329100000 -0.8929520000
C -3.8261340000 -1.9063300000 0.2552620000
C -2.5009950000 -1.4849400000 0.0629190000
C -4.0658730000 -3.1973330000 0.7423780000
C -2.9812160000 -4.0365700000 1.0264750000
C -1.6872870000 -3.5570470000 0.7955100000
N -1.4566750000 -2.3160990000 0.3261340000
C 1.1994180000 1.5995600000 -0.2848220000
C 1.5033410000 3.1099740000 -0.2479930000
C 2.0549380000 0.9083880000 -1.3784860000
C 1.5493420000 0.9477180000 1.0858390000
N 1.3633320000 -0.3884330000 1.2252520000
C 1.6490110000 -1.0029490000 2.3931720000
C 2.1432810000 -0.3109440000 3.5003730000
C 2.3453720000 1.0667630000 3.3763460000
C 2.0473370000 1.7001880000 2.1619000000
C 2.9701560000 1.6199670000 -2.1740780000
C 3.7647050000 0.9328630000 -3.1001710000
C 3.6424190000 -0.4566760000 -3.2090820000
C 2.7106110000 -1.0995630000 -2.3934970000
N 1.9291540000 -0.4313200000 -1.5157870000
H -3.2549910000 2.9691920000 -1.2663370000
H -5.0925630000 -3.5398520000 0.9023760000
H -3.1260670000 -5.0476280000 1.4154840000
H -0.8026820000 -4.1727610000 0.9857530000
H 0.8882570000 3.6106810000 0.5147140000
H 2.5629640000 3.2901390000 -0.0135990000
H 1.2865910000 3.5753090000 -1.2211330000
H 1.4728720000 -2.0835480000 2.4253130000
H 2.3633620000 -0.8463430000 4.4278750000
H 2.7333070000 1.6533570000 4.2148920000
H 2.2073570000 2.7745260000 2.0669910000
H 3.0759340000 2.7005840000 -2.0738130000
H 4.4800530000 1.4836100000 -3.7190850000
H 4.2544230000 -1.0381120000 -3.9041690000
H 2.5802050000 -2.1865590000 -2.4186810000

Fe 0.4907530000 -1.6062340000 -0.3587940000
H -0.8222850000 3.4427310000 -1.0718580000
N 1.5320150000 -3.1738610000 -0.0729930000
H 1.3049880000 -4.1190450000 -0.4065540000
H 2.4148690000 -3.2360040000 0.4487550000
N -0.3303210000 -2.1936330000 -2.3324250000
H -1.0982830000 -1.5933430000 -2.6597360000
H -0.7043010000 -3.1509740000 -2.3147500000
H 0.3685780000 -2.1815270000 -3.0858050000
H -4.6609010000 -1.2359360000 0.0386420000
H -4.1243080000 0.6867520000 -0.7173320000

[(bpyPy₂Me)Fe(NH₃)(NH₂)]²⁺, multiplicity = 2

C -2.5814980000 2.2060830000 -0.8621380000
C -3.0507210000 0.9114080000 -0.6133070000
C -2.1109740000 -0.1078200000 -0.4099400000
N -0.7809720000 0.1567660000 -0.5162310000
C -0.3096100000 1.4144360000 -0.6059720000
C -1.2053890000 2.4749750000 -0.8120330000
C -3.6599670000 -1.9994760000 0.2887560000
C -2.3804620000 -1.4744320000 0.0570630000
C -3.7849200000 -3.2780730000 0.8417110000
C -2.6222730000 -3.9963810000 1.1501030000
C -1.3761790000 -3.4234320000 0.8778980000
N -1.2432900000 -2.1910340000 0.3436350000
C 1.2015030000 1.5747590000 -0.3284180000
C 1.5762860000 3.0653770000 -0.2910440000
C 2.0317370000 0.8170770000 -1.3810450000
C 1.4611930000 0.8944100000 1.0446620000
N 1.0995380000 -0.4109440000 1.1725980000
C 1.2394120000 -1.0288920000 2.3675600000
C 1.7884540000 -0.3956660000 3.4818880000
C 2.1988740000 0.9349510000 3.3548860000
C 2.0234620000 1.5856310000 2.1275310000
C 3.0001810000 1.4501010000 -2.1746170000
C 3.7439140000 0.7054590000 -3.0972950000
C 3.5001490000 -0.6671800000 -3.2072930000
C 2.5229160000 -1.2373830000 -2.3930200000
N 1.8019550000 -0.5170390000 -1.4954570000
H -3.2890290000 3.0205150000 -1.0421770000
H -4.7741700000 -3.7046780000 1.0296990000
H -2.6663210000 -4.9965460000 1.5877850000
H -0.4589020000 -3.9766280000 1.0903210000
H 0.9903980000 3.5920880000 0.4769150000
H 2.6442790000 3.1968210000 -0.0618650000

H 1.3724360000 3.5378510000 -1.2642010000
 H 0.8870400000 -2.0618370000 2.4336350000
 H 1.8828900000 -0.9432720000 4.4232850000
 H 2.6395810000 1.4702280000 4.2011890000
 H 2.3234110000 2.6285300000 2.0218600000
 H 3.1773430000 2.5213030000 -2.0748350000
 H 4.5005350000 1.1961530000 -3.7169620000
 H 4.0505830000 -1.2982050000 -3.9103570000
 H 2.2876420000 -2.3023590000 -2.4640920000
 Fe 0.3748430000 -1.3769330000 -0.4458040000
 H -0.8445770000 3.4982680000 -0.9196940000
 N 1.6034550000 -2.9434660000 -0.0440470000
 H 1.3813060000 -3.7345280000 -0.6607610000
 H 1.5671050000 -3.3104720000 0.9154240000
 N -0.2345790000 -2.0924510000 -2.0220480000
 H 0.0938490000 -1.7567580000 -2.9346900000
 H -1.1635580000 -2.5165560000 -2.1277170000
 H -4.5454980000 -1.4095770000 0.0406690000
 H -4.1217670000 0.7041560000 -0.5529750000
 H 2.5957150000 -2.7210270000 -0.2008960000

[(bpyPy₂Me)Fe(NH₃)(NH₂)]²⁺, multiplicity = 4

C -2.5749440000 2.2152240000 -0.9192620000
 C -3.0598310000 0.9353710000 -0.6237580000
 C -2.1279550000 -0.0804940000 -0.3615070000
 N -0.8049290000 0.1796310000 -0.4267610000
 C -0.3203010000 1.4177900000 -0.5901260000
 C -1.1976500000 2.4789440000 -0.8719800000
 C -3.7480960000 -1.9175690000 0.3248200000
 C -2.4425590000 -1.4526770000 0.1014410000
 C -3.9373710000 -3.2081880000 0.8314760000
 C -2.8160960000 -4.0025620000 1.1022040000
 C -1.5439320000 -3.4799230000 0.8430830000
 N -1.3571800000 -2.2362720000 0.3617800000
 C 1.2008030000 1.5714070000 -0.3241000000
 C 1.5617090000 3.0670950000 -0.2633540000
 C 2.0301790000 0.8588500000 -1.4176670000
 C 1.4864640000 0.8774070000 1.0398560000
 N 1.1827620000 -0.4440680000 1.1749620000
 C 1.3435190000 -1.0528930000 2.3720840000
 C 1.8517700000 -0.3942390000 3.4910310000
 C 2.2038610000 0.9519560000 3.3607800000
 C 2.0105270000 1.5900770000 2.1292940000
 C 2.9389550000 1.5452560000 -2.2391900000
 C 3.6994900000 0.8375910000 -3.1780180000

C 3.5373730000 -0.5476150000 -3.2864590000
 C 2.6010250000 -1.1674130000 -2.4600660000
 N 1.8704140000 -0.4803780000 -1.5507570000
 H -3.2748050000 3.0250080000 -1.1458820000
 H -4.9479240000 -3.5865160000 1.0114450000
 H -2.9138030000 -5.0157100000 1.5011840000
 H -0.6470810000 -4.0799490000 1.0220970000
 H 0.9707840000 3.5752260000 0.5136330000
 H 2.6297680000 3.2081470000 -0.0398960000
 H 1.3462490000 3.5531000000 -1.2266360000
 H 1.0463700000 -2.1027070000 2.4298400000
 H 1.9636250000 -0.9351230000 4.4342380000
 H 2.6154650000 1.5102050000 4.2070210000
 H 2.2669630000 2.6446050000 2.0270850000
 H 3.0620900000 2.6249360000 -2.1520400000
 H 4.4121380000 1.3701840000 -3.8152180000
 H 4.1132290000 -1.1433650000 -3.9994900000
 H 2.4083390000 -2.2425860000 -2.5216510000
 Fe 0.4835820000 -1.4949610000 -0.4227410000
 H -0.8307770000 3.4928070000 -1.0378980000
 N 1.7922760000 -3.1532340000 0.1209950000
 H 1.7333250000 -3.8621370000 -0.6199790000
 H 1.6242100000 -3.6568610000 1.0008510000
 N -0.1037420000 -2.2798830000 -1.9677340000
 H 0.0897030000 -1.8382650000 -2.8750330000
 H -1.0087940000 -2.7611240000 -2.0132400000
 H -4.6058650000 -1.2761160000 0.1091400000
 H -4.1345980000 0.7439130000 -0.5832460000
 H 2.7766890000 -2.8584840000 0.1644980000

[(bpyPy₂Me)Fe(NH₃)(NH₂)]²⁺, multiplicity = 6

C -2.5751695026 2.1727958726 -0.9295395171
 C -3.0615640728 0.8987442183 -0.6202083321
 C -2.1359164992 -0.1106654020 -0.3163891703
 N -0.8046592568 0.1408547671 -0.3442386318
 C -0.3218313873 1.3811651786 -0.5370572059
 C -1.2002710230 2.4312456921 -0.8617081414
 C -3.8303073578 -1.9103913103 0.2766925453
 C -2.5035948080 -1.4781599589 0.1224085996
 C -4.0779561074 -3.2023672486 0.7555195776
 C -2.9958705735 -4.0328286528 1.0711113210
 C -1.6996215351 -3.5408108582 0.8822496946
 N -1.4582961942 -2.2986971931 0.4223910234
 C 1.1993151418 1.5960423158 -0.2925861610
 C 1.5003661858 3.1073016305 -0.2613830559

C 2.0444138299 0.9093139538 -1.3924084518
 C 1.5593118428 0.9435715342 1.0748865678
 N 1.3830095488 -0.3949253637 1.2111758486
 C 1.6551973822 -0.9878264863 2.3925125208
 C 2.1323795999 -0.2879812656 3.5023003518
 C 2.3348004328 1.0883777760 3.3714096743
 C 2.0436942344 1.7081408825 2.1491852592
 C 2.9838071585 1.6110697534 -2.1675595550
 C 3.7536336443 0.9245771445 -3.1151034072
 C 3.5736407459 -0.4532443158 -3.2758862428
 C 2.6150437151 -1.0863444041 -2.4839827050
 N 1.8735537817 -0.4205968176 -1.5702589709
 H -3.2690749409 2.9773567655 -1.1898442564
 H -5.1066769520 -3.5525584372 0.8822496123
 H -3.1426277420 -5.0458248667 1.4541162465
 H -0.8278274110 -4.1629351778 1.1056805892
 H 0.8856436764 3.6107199616 0.4995920703
 H 2.5595492701 3.2909637244 -0.0281630243
 H 1.2818490821 3.5672205380 -1.2369211570
 H 1.4778487437 -2.0652871910 2.4539167066
 H 2.3382394990 -0.8177637019 4.4362549245
 H 2.7123029960 1.6829548969 4.2089662091
 H 2.1962292082 2.7827702291 2.0465356059
 H 3.1255473431 2.6841784966 -2.0371807391
 H 4.4871655241 1.4685468535 -3.7184235766
 H 4.1530117401 -1.0318383001 -4.0004938881
 H 2.4112832547 -2.1576900480 -2.5822595037
 Fe 0.4457123925 -1.6071061491 -0.4149627384
 H -0.8305545359 3.4391332478 -1.0499385229
 N 1.6266342585 -3.3362101446 0.1533965932
 H 1.4180436029 -4.1193578638 -0.4792077232
 H 1.5622239939 -3.7212797572 1.1044434172
 N -0.1456260359 -2.3178302108 -2.1073372628
 H 0.0186494639 -1.9247140751 -3.0422326327
 H -0.7372504561 -3.1519051792 -2.2173083241
 H -4.6622128834 -1.2470183763 0.0297912067
 H -4.1360033263 0.7022864025 -0.6093353794
 H 2.6262343077 -3.1317550798 0.0162811114

[(bpyPy₂Me)Fe(MeCN)(NH₃)]³⁺, multiplicity = 2

C -2.5752200000 2.1884830000 -0.9954320000
 C -3.0279790000 0.8939750000 -0.7222740000
 C -2.0773860000 -0.1008500000 -0.4668970000
 N -0.7450320000 0.1823460000 -0.5532910000
 C -0.2949970000 1.4496970000 -0.6602260000

C -1.2061550000 2.4835500000 -0.9165180000
C -3.5954380000 -1.9989320000 0.2898250000
C -2.3316060000 -1.4534700000 0.0328170000
C -3.6814860000 -3.2734270000 0.8602520000
C -2.5027230000 -3.9706330000 1.1561570000
C -1.2701180000 -3.3862680000 0.8535050000
N -1.1835430000 -2.1534770000 0.3091460000
C 1.1998170000 1.6526520000 -0.3447630000
C 1.5381250000 3.1510320000 -0.2942320000
C 2.0695060000 0.9152720000 -1.3763110000
C 1.4466540000 0.9720340000 1.0289840000
N 1.1519370000 -0.3510060000 1.1315870000
C 1.3265020000 -1.0091980000 2.3012640000
C 1.8180700000 -0.3680350000 3.4371480000
C 2.1409290000 0.9894050000 3.3507280000
C 1.9521350000 1.6628990000 2.1372590000
C 3.0409690000 1.5641920000 -2.1495350000
C 3.8235780000 0.8262810000 -3.0447990000
C 3.6213470000 -0.5540730000 -3.1483430000
C 2.6393510000 -1.1435870000 -2.3573930000
N 1.8798790000 -0.4237230000 -1.4925910000
H -3.2916890000 2.9846900000 -1.2156680000
H -4.6590700000 -3.7158460000 1.0711510000
H -2.5233390000 -4.9647980000 1.6094110000
H -0.3335590000 -3.9120480000 1.0482900000
H 0.9157830000 3.6605060000 0.4566980000
H 2.5953750000 3.3027860000 -0.0317800000
H 1.3546730000 3.6196010000 -1.2726660000
H 1.0633950000 -2.0694380000 2.3197640000
H 1.9421490000 -0.9362300000 4.3622890000
H 2.5356020000 1.5274590000 4.2175090000
H 2.1980290000 2.7222890000 2.0596320000
H 3.1889470000 2.6401850000 -2.0568300000
H 4.5819860000 1.3292730000 -3.6518770000
H 4.2075870000 -1.1762000000 -3.8291310000
H 2.4472780000 -2.2167830000 -2.4125990000
Fe 0.4425640000 -1.3108620000 -0.4394630000
H -0.8603850000 3.5104700000 -1.0392620000
N 1.5818950000 -2.8424020000 -0.1667190000
N -0.2306230000 -2.0848560000 -2.1838530000
H -1.2566370000 -2.1241350000 -2.2547460000
H 0.1013940000 -3.0480870000 -2.3257180000
H 0.0839150000 -1.5380510000 -2.9964010000
H -4.4964430000 -1.4287700000 0.0524950000
H -4.0953180000 0.6665370000 -0.6811910000
C 2.2968210000 -3.7429520000 0.0213640000

C 3.1854390000 -4.8625520000 0.2515740000
H 3.2041990000 -5.0897370000 1.3309850000
H 4.2003000000 -4.5959910000 -0.0881480000
H 2.8192410000 -5.7395120000 -0.3077100000

[(bpyPy₂Me)Fe(MeCN)(NH₃)]³⁺, multiplicity = 4

C -2.5652790000 2.1266200000 -1.0758820000
C -3.0267520000 0.8460270000 -0.7538270000
C -2.0902080000 -0.1388000000 -0.4188830000
N -0.7599790000 0.1530280000 -0.4473190000
C -0.2985850000 1.4100250000 -0.6266620000
C -1.2002910000 2.4256650000 -0.9795160000
C -3.7227240000 -1.9788100000 0.2363800000
C -2.4173960000 -1.4926800000 0.0780450000
C -3.9056340000 -3.2574960000 0.7801440000
C -2.7868990000 -4.0137560000 1.1502840000
C -1.5121160000 -3.4703060000 0.9503350000
N -1.3370730000 -2.2413560000 0.4316860000
C 1.2008780000 1.6592380000 -0.3317980000
C 1.4708110000 3.1733690000 -0.2608290000
C 2.0924430000 1.0013080000 -1.4130670000
C 1.5232140000 0.9840960000 1.0301160000
N 1.2811890000 -0.3491980000 1.1732550000
C 1.5248070000 -0.9895510000 2.3426540000
C 2.0379550000 -0.3165610000 3.4486350000
C 2.3164020000 1.0475660000 3.3242120000
C 2.0582310000 1.6978530000 2.1097020000
C 2.9853190000 1.7253760000 -2.2149810000
C 3.7981320000 1.0405160000 -3.1284300000
C 3.7116780000 -0.3530450000 -3.2175420000
C 2.7924260000 -1.0104500000 -2.4005370000
N 2.0007550000 -0.3428940000 -1.5326520000
H -3.2751470000 2.9091980000 -1.3580650000
H -4.9159300000 -3.6553690000 0.9121640000
H -2.8884920000 -5.0124120000 1.5828600000
H -0.6092160000 -4.0315970000 1.2088330000
H 0.8406080000 3.6432220000 0.5091430000
H 2.5263610000 3.3673560000 -0.0205070000
H 1.2504160000 3.6483940000 -1.2279240000
H 1.2960340000 -2.0569250000 2.3795240000
H 2.2159500000 -0.8647350000 4.3769250000
H 2.7310700000 1.6121570000 4.1644450000
H 2.2728700000 2.7619540000 2.0119150000
H 3.0573430000 2.8103020000 -2.1340780000
H 4.4985290000 1.5977940000 -3.7577060000

H 4.3383740000 -0.9281840000 -3.9038750000
 H 2.6891730000 -2.0992140000 -2.4331770000
 Fe 0.5245800000 -1.3504280000 -0.3336980000
 H -0.8498190000 3.4413060000 -1.1641310000
 N 1.6055050000 -2.9639880000 -0.0023580000
 N -0.1009330000 -2.1346350000 -2.1081150000
 H -1.0090850000 -2.6098120000 -2.0209790000
 H 0.5441660000 -2.8421820000 -2.4843460000
 H -0.2132240000 -1.4142900000 -2.8344290000
 H -4.5837820000 -1.3728520000 -0.0541450000
 H -4.0956690000 0.6234920000 -0.7438170000
 C 2.2752690000 -3.9094520000 0.1254800000
 C 3.1070320000 -5.0813190000 0.2868900000
 H 3.1925590000 -5.3173900000 1.3610170000
 H 4.1079370000 -4.8673020000 -0.1255290000
 H 2.6528430000 -5.9291880000 -0.2523700000

[(bpyPy₂Me)Fe(MeCN)(NH₃)]³⁺, multiplicity = 6

C -2.5959630000 2.1666360000 -0.9796670000
 C -3.0549660000 0.8780640000 -0.6868670000
 C -2.1100880000 -0.1080370000 -0.3783730000
 N -0.7824690000 0.1847340000 -0.3981580000
 C -0.3235220000 1.4410190000 -0.5733580000
 C -1.2288610000 2.4643400000 -0.8957020000
 C -3.7321670000 -1.9605360000 0.2550180000
 C -2.4298460000 -1.4840880000 0.0567290000
 C -3.9146180000 -3.2645000000 0.7348990000
 C -2.7948710000 -4.0601600000 1.0056110000
 C -1.5219050000 -3.5308880000 0.7721100000
 N -1.3468270000 -2.2749680000 0.3121530000
 C 1.1849260000 1.6863570000 -0.3108170000
 C 1.4644770000 3.2008020000 -0.2902840000
 C 2.0539440000 0.9929590000 -1.3877350000
 C 1.5431610000 1.0493350000 1.0633460000
 N 1.3701730000 -0.2899390000 1.2106210000
 C 1.6576630000 -0.9018150000 2.3823490000
 C 2.1436010000 -0.1974700000 3.4836710000
 C 2.3364010000 1.1805530000 3.3516450000
 C 2.0337670000 1.8080640000 2.1341700000
 C 2.9872980000 1.6902110000 -2.1685760000
 C 3.7946460000 0.9907310000 -3.0749660000
 C 3.6633690000 -0.3976320000 -3.1846230000
 C 2.7052030000 -1.0315320000 -2.3960030000
 N 1.9207480000 -0.3483560000 -1.5292640000
 H -3.3085290000 2.9551800000 -1.2377660000

H -4.9251400000 -3.6504510000 0.8967910000
 H -2.8936350000 -5.0793100000 1.3876830000
 H -0.6199940000 -4.1211910000 0.9540950000
 H 0.8397870000 3.6979630000 0.4668810000
 H 2.5205020000 3.3980060000 -0.0552650000
 H 1.2423840000 3.6484900000 -1.2702020000
 H 1.4928330000 -1.9822830000 2.4291020000
 H 2.3647610000 -0.7278190000 4.4132550000
 H 2.7200220000 1.7739570000 4.1870010000
 H 2.1820730000 2.8832090000 2.0331860000
 H 3.0963310000 2.7706210000 -2.0734450000
 H 4.5235470000 1.5330650000 -3.6846410000
 H 4.2802240000 -0.9860600000 -3.8684500000
 H 2.5567360000 -2.1140340000 -2.4534120000
 Fe 0.5143880000 -1.4522870000 -0.3579720000
 H -0.8848320000 3.4843290000 -1.0672790000
 N 1.6356250000 -3.1278410000 0.0690210000
 N -0.1563390000 -2.1692850000 -2.3144570000
 H -1.1739200000 -2.3175210000 -2.3450330000
 H 0.2589980000 -3.0771340000 -2.5658290000
 H 0.0570000000 -1.5259650000 -3.0881230000
 H -4.5938720000 -1.3229370000 0.0462180000
 H -4.1232040000 0.6522640000 -0.6883220000
 C 2.3293490000 -4.0555630000 0.2101240000
 C 3.1886610000 -5.2016340000 0.3873350000
 H 3.2745530000 -5.4226590000 1.4648930000
 H 4.1842150000 -4.9715180000 -0.0291500000
 H 2.7508290000 -6.0657960000 -0.1406960000

[(bpyPy₂Me)Fe(NH₃)(NHNH₂)]²⁺, multiplicity = 2

C -2.5496380000 2.1879910000 -1.0197640000
 C -3.0083550000 0.8844470000 -0.7958490000
 C -2.0641170000 -0.1218330000 -0.5501080000
 N -0.7286550000 0.1558850000 -0.6089910000
 C -0.2793910000 1.4270080000 -0.6612180000
 C -1.1805060000 2.4759000000 -0.8983000000
 C -3.6107860000 -2.0053310000 0.1794100000
 C -2.3312090000 -1.4734320000 -0.0410100000
 C -3.7405250000 -3.2464570000 0.8112220000
 C -2.5813510000 -3.9217100000 1.2171330000
 C -1.3343150000 -3.3477250000 0.9502350000
 N -1.1938310000 -2.1579740000 0.3239560000
 C 1.2196960000 1.5988920000 -0.3318300000
 C 1.5783200000 3.0921770000 -0.2614460000
 C 2.0732940000 0.8686850000 -1.3825780000

C 1.4600810000 0.8946490000 1.0322440000
 N 1.1424450000 -0.4294090000 1.1226090000
 C 1.2991550000 -1.0688270000 2.3066350000
 C 1.8060440000 -0.4423680000 3.4437680000
 C 2.1599140000 0.9084250000 3.3577890000
 C 1.9773980000 1.5790080000 2.1424750000
 C 3.0502220000 1.5198240000 -2.1516750000
 C 3.8014000000 0.7978220000 -3.0860120000
 C 3.5526820000 -0.5712440000 -3.2324700000
 C 2.5689670000 -1.1598780000 -2.4399950000
 N 1.8411470000 -0.4633860000 -1.5261100000
 H -3.2601650000 2.9923390000 -1.2308240000
 H -4.7307230000 -3.6751910000 0.9896780000
 H -2.6284790000 -4.8886140000 1.7240240000
 H -0.4179360000 -3.8688490000 1.2398190000
 H 0.9655510000 3.6027060000 0.4966740000
 H 2.6383540000 3.2316640000 -0.0017560000
 H 1.3956090000 3.5770380000 -1.2327750000
 H 0.9944210000 -2.1178870000 2.3384790000
 H 1.9142880000 -1.0105830000 4.3715980000
 H 2.5659190000 1.4403650000 4.2234090000
 H 2.2390760000 2.6349230000 2.0659590000
 H 3.2270890000 2.5882140000 -2.0230900000
 H 4.5652080000 1.3010470000 -3.6865390000
 H 4.1062400000 -1.1861410000 -3.9475040000
 H 2.3402880000 -2.2235220000 -2.5390950000
 Fe 0.4287240000 -1.3398260000 -0.4758980000
 H -0.8304120000 3.5057940000 -0.9792350000
 N 1.6302770000 -2.9514850000 -0.1790830000
 H 1.4726290000 -3.6878540000 -0.8826940000
 H 1.5411870000 -3.4239260000 0.7295640000
 N -0.1879550000 -2.0947890000 -2.1219910000
 N -0.4392110000 -3.4039800000 -2.3632170000
 H -0.0550330000 -1.6020560000 -3.0141340000
 H 2.6282840000 -2.7096300000 -0.2438150000
 H -4.4951820000 -1.4456760000 -0.1349240000
 H -4.0780700000 0.6610390000 -0.7822150000
 H -0.8600010000 -3.6149960000 -3.2736490000
 H -0.8992090000 -3.8921550000 -1.5880770000

[(bpyPy₂Me)Fe(NH₃)(NHNH₂)]²⁺, multiplicity = 4

C -2.5264280000 2.1720960000 -1.0319420000
 C -3.0142800000 0.8955150000 -0.7316900000
 C -2.0951900000 -0.1174970000 -0.4232080000
 N -0.7600420000 0.1343920000 -0.4441010000

C -0.2787540000 1.3838280000 -0.6034250000
C -1.1538490000 2.4333350000 -0.9355950000
C -3.7893350000 -1.9502020000 0.0666630000
C -2.4670770000 -1.4749170000 0.0442870000
C -4.0478530000 -3.2211900000 0.5937940000
C -2.9809050000 -3.9807580000 1.0904400000
C -1.6890590000 -3.4411170000 1.0245760000
N -1.4327070000 -2.2238420000 0.5131810000
C 1.2329750000 1.5921230000 -0.3201190000
C 1.5334640000 3.1008390000 -0.2292750000
C 2.0920560000 0.9447320000 -1.4357060000
C 1.5578710000 0.8916540000 1.0299240000
N 1.2706940000 -0.4349550000 1.1628920000
C 1.4931950000 -1.0540600000 2.3478830000
C 2.0379610000 -0.4018300000 3.4518210000
C 2.3658160000 0.9515460000 3.3237050000
C 2.1174920000 1.5979170000 2.1073460000
C 3.0079130000 1.6740420000 -2.2137440000
C 3.7636050000 1.0080720000 -3.1876760000
C 3.5874610000 -0.3684570000 -3.3695670000
C 2.6501680000 -1.0222610000 -2.5672230000
N 1.9282500000 -0.3802840000 -1.6251790000
H -3.2181910000 2.9765460000 -1.2983080000
H -5.0702450000 -3.6104600000 0.6157150000
H -3.1364260000 -4.9744280000 1.5187670000
H -0.8300360000 -4.0071120000 1.4024800000
H 0.9200340000 3.5745440000 0.5519660000
H 2.5935000000 3.2760940000 0.0060600000
H 1.3149000000 3.5963060000 -1.1870490000
H 1.2122780000 -2.1090010000 2.4060710000
H 2.1971720000 -0.9515380000 4.3832630000
H 2.8030260000 1.5062180000 4.1594250000
H 2.3619360000 2.6552640000 2.0056230000
H 3.1410330000 2.7469750000 -2.0698760000
H 4.4819850000 1.5660630000 -3.7966050000
H 4.1562970000 -0.9285290000 -4.1170100000
H 2.4604980000 -2.0951190000 -2.6786440000
Fe 0.5031360000 -1.4444210000 -0.3592320000
H -0.7808370000 3.4427340000 -1.1101270000
N 1.7307960000 -3.0762850000 -0.0747630000
H 1.6094890000 -3.7431760000 -0.8533460000
H 1.5557670000 -3.6171530000 0.7827930000
N -0.1485560000 -2.2681520000 -1.9392050000
N -0.2261200000 -3.6173340000 -2.1651760000
H -0.0432890000 -1.7819140000 -2.8389680000
H 2.7293620000 -2.8312370000 -0.0383930000

H -4.6070000000 -1.3392660000 -0.3233100000
H -4.0892680000 0.7008760000 -0.7178760000
H -0.5816120000 -3.8653360000 -3.0947310000
H -0.7442200000 -4.1107750000 -1.4287970000

[(bpyPy₂Me)Fe(NH₃)(NHNH₂)]²⁺, multiplicity = 6

C -2.5552740000 2.1671830000 -0.9621470000
C -3.0265410000 0.8809750000 -0.6847880000
C -2.0915730000 -0.1236540000 -0.3894580000
N -0.7598510000 0.1395250000 -0.3999700000
C -0.2952440000 1.3942720000 -0.5622050000
C -1.1836460000 2.4397500000 -0.8714430000
C -3.7826740000 -1.9410910000 0.1497490000
C -2.4546310000 -1.4974860000 0.0292880000
C -4.0357330000 -3.2356970000 0.6161490000
C -2.9548850000 -4.0591860000 0.9568370000
C -1.6586760000 -3.5553260000 0.8042810000
N -1.4078180000 -2.3101830000 0.3510030000
C 1.2215810000 1.6276220000 -0.3062340000
C 1.5093870000 3.1417560000 -0.2873780000
C 2.0835530000 0.9389060000 -1.3934040000
C 1.5799740000 0.9953710000 1.0729900000
N 1.4323290000 -0.3456600000 1.2181310000
C 1.7253270000 -0.9270490000 2.4014280000
C 2.1859360000 -0.2102360000 3.5067440000
C 2.3473090000 1.1721220000 3.3710090000
C 2.0411610000 1.7779750000 2.1458020000
C 3.0343420000 1.6420640000 -2.1545580000
C 3.8158440000 0.9569220000 -3.0933610000
C 3.6360900000 -0.4205450000 -3.2590360000
C 2.6663190000 -1.0528140000 -2.4795130000
N 1.9125630000 -0.3905310000 -1.5741580000
H -3.2562140000 2.9683420000 -1.2141550000
H -5.0649840000 -3.5933160000 0.7151350000
H -3.1036360000 -5.0747670000 1.3325220000
H -0.7891730000 -4.1695530000 1.0585200000
H 0.8848140000 3.6481790000 0.4634840000
H 2.5647870000 3.3375390000 -0.0463450000
H 1.2948820000 3.5906280000 -1.2691570000
H 1.5794250000 -2.0104500000 2.4628330000
H 2.4110670000 -0.7299660000 4.4420580000
H 2.7079170000 1.7802550000 4.2063440000
H 2.1665950000 2.8558180000 2.0385280000
H 3.1753370000 2.7149590000 -2.0213590000
H 4.5579110000 1.5011850000 -3.6860270000

H 4.2246140000 -0.9981000000 -3.9772090000
 H 2.4667600000 -2.1248020000 -2.5812360000
 Fe 0.5191620000 -1.5668340000 -0.3568110000
 H -0.8253190000 3.4562700000 -1.0340180000
 N 1.6819680000 -3.3565960000 0.0745070000
 H 1.5086930000 -4.1013290000 -0.6142540000
 H 1.5940240000 -3.8098180000 0.9937100000
 N -0.1061910000 -2.3116700000 -2.2060950000
 N -0.5044880000 -3.5632680000 -2.5375830000
 H -0.0030510000 -1.7639880000 -3.0702470000
 H 2.6837380000 -3.1362170000 -0.0116640000
 H -4.6126740000 -1.2818710000 -0.1142900000
 H -4.0985210000 0.6707920000 -0.6887160000
 H -1.0192110000 -3.6659050000 -3.4182080000
 H -0.9245440000 -4.0913940000 -1.7672130000

[(bpyPy₂Me)Fe(NH₂NH)(NH₃)]²⁺, multiplicity = 2

C -2.5622260000 2.2256970000 -0.9490980000
 C -3.0164990000 0.9215810000 -0.7258320000
 C -2.0673650000 -0.0878320000 -0.5115780000
 N -0.7309750000 0.1838220000 -0.6036510000
 C -0.2853410000 1.4579620000 -0.6533860000
 C -1.1894560000 2.5098450000 -0.8573410000
 C -3.5946040000 -1.9844080000 0.2387660000
 C -2.3239230000 -1.4474970000 -0.0184720000
 C -3.6967510000 -3.2417480000 0.8423330000
 C -2.5206110000 -3.9270460000 1.1788540000
 C -1.2849600000 -3.3480500000 0.8764270000
 N -1.1737860000 -2.1404060000 0.2793400000
 C 1.2179210000 1.6250530000 -0.3456890000
 C 1.5794180000 3.1168630000 -0.2582810000
 C 2.0585080000 0.9103650000 -1.4174260000
 C 1.4709000000 0.9029320000 1.0087380000
 N 1.1752270000 -0.4280070000 1.0813400000
 C 1.3489590000 -1.0898330000 2.2518500000
 C 1.8381440000 -0.4679290000 3.3994690000
 C 2.1634370000 0.8915720000 3.3363590000
 C 1.9743180000 1.5782570000 2.1310010000
 C 2.9997540000 1.5781960000 -2.2157230000
 C 3.7481920000 0.8650320000 -3.1590900000
 C 3.5431660000 -0.5142430000 -3.2766240000
 C 2.5952860000 -1.1209660000 -2.4551060000
 N 1.8560780000 -0.4280660000 -1.5472540000
 H -3.2763100000 3.0332560000 -1.1343580000
 H -4.6785840000 -3.6754570000 1.0531730000

H -2.5486400000 -4.9061190000 1.6647180000
 H -0.3490410000 -3.8632540000 1.1094510000
 H 0.9776270000 3.6174610000 0.5154060000
 H 2.6434950000 3.2507290000 -0.0115640000
 H 1.3837350000 3.6162210000 -1.2195830000
 H 1.0860270000 -2.1501280000 2.2451210000
 H 1.9589640000 -1.0480600000 4.3182760000
 H 2.5555070000 1.4180040000 4.2118130000
 H 2.2177550000 2.6396380000 2.0713900000
 H 3.1506940000 2.6526970000 -2.1059960000
 H 4.4807410000 1.3820930000 -3.7861240000
 H 4.1061000000 -1.1227550000 -3.9896000000
 H 2.4092200000 -2.1972900000 -2.5033700000
 Fe 0.4460430000 -1.3158680000 -0.5046280000
 H -0.8406720000 3.5407950000 -0.9329080000
 N 1.5114070000 -2.8759040000 -0.2944060000
 H 1.1821890000 -3.8277210000 -0.4977500000
 N -0.2911110000 -2.0701450000 -2.2476690000
 H -1.2654410000 -1.7902160000 -2.4276510000
 H -0.2892330000 -3.0976500000 -2.2940050000
 H 0.2328520000 -1.7544420000 -3.0741420000
 N 2.7663320000 -2.9448440000 0.2185500000
 H -4.4907320000 -1.4159230000 -0.0225540000
 H -4.0855110000 0.6987680000 -0.6860630000
 H 3.3212070000 -3.7603270000 -0.0595280000
 H 3.2824010000 -2.0621020000 0.1734480000

[(bpyPy₂Me)Fe(NHNH₂)(NH₃)]²⁺, multiplicity = 4

C -2.5639220000 2.1565130000 -0.8642230000
 C -3.0063490000 0.8566760000 -0.6062010000
 C -2.0505400000 -0.1427210000 -0.3805060000
 N -0.7125590000 0.1343180000 -0.4571080000
 C -0.2718360000 1.4096560000 -0.5807530000
 C -1.1926330000 2.4441850000 -0.8125870000
 C -3.6332940000 -2.0311230000 0.2588590000
 C -2.3432420000 -1.5195710000 0.0419920000
 C -3.7762730000 -3.3309700000 0.7537300000
 C -2.6273330000 -4.0884250000 1.0261000000
 C -1.3737370000 -3.5287690000 0.7674170000
 N -1.2286560000 -2.2781130000 0.2793080000
 C 1.2397220000 1.6580820000 -0.3499740000
 C 1.5212600000 3.1721270000 -0.3317780000
 C 2.0933290000 0.9668500000 -1.4382100000
 C 1.5974910000 1.0220210000 1.0280050000
 N 1.3735670000 -0.3072940000 1.1834340000

C 1.6077590000 -0.8925160000 2.3792160000
 C 2.1039440000 -0.1890260000 3.4777670000
 C 2.3715470000 1.1753310000 3.3230530000
 C 2.1132660000 1.7852010000 2.0889940000
 C 3.0327570000 1.6643430000 -2.2176600000
 C 3.7982550000 0.9698850000 -3.1617410000
 C 3.6196160000 -0.4110900000 -3.3026170000
 C 2.6725580000 -1.0389930000 -2.4935250000
 N 1.9246140000 -0.3652210000 -1.5923420000
 H -3.2835560000 2.9556120000 -1.0637110000
 H -4.7732750000 -3.7452300000 0.9302660000
 H -2.6937550000 -5.1039090000 1.4256970000
 H -0.4537010000 -4.0900330000 0.9542510000
 H 0.9172200000 3.6723770000 0.4402140000
 H 2.5823520000 3.3687940000 -0.1188870000
 H 1.2806170000 3.6231050000 -1.3063680000
 H 1.3961110000 -1.9651940000 2.4435030000
 H 2.2763000000 -0.7077880000 4.4247680000
 H 2.7719460000 1.7670790000 4.1520230000
 H 2.3125550000 2.8501310000 1.9654490000
 H 3.1734560000 2.7387060000 -2.0960120000
 H 4.5284730000 1.5068330000 -3.7752760000
 H 4.1991910000 -0.9967790000 -4.0215320000
 H 2.4962580000 -2.1175660000 -2.5452500000
 Fe 0.4814360000 -1.3997230000 -0.4195650000
 H -0.8528860000 3.4717800000 -0.9437170000
 N 1.4944720000 -2.9873000000 -0.4513790000
 H 1.0774400000 -3.7981900000 -0.9275030000
 N -0.3354740000 -2.0309360000 -2.4843840000
 H -1.3504360000 -2.1948010000 -2.4913580000
 H 0.0745830000 -2.8818250000 -2.8906140000
 H -0.1759370000 -1.2923540000 -3.1809820000
 N 2.2638600000 -3.4380540000 0.5797660000
 H -4.5125530000 -1.4167480000 0.0510490000
 H -4.0731290000 0.6248530000 -0.5672800000
 H 2.5950680000 -4.4025620000 0.4810110000
 H 3.0138820000 -2.7890320000 0.8365400000

[(bpyPy₂Me)Fe(NHNH₂)(NH₃)]²⁺, multiplicity = 6

C -2.5581420000 2.1780390000 -0.9619830000
 C -3.0290380000 0.8925020000 -0.6793410000
 C -2.0931010000 -0.1070110000 -0.3697740000
 N -0.7628600000 0.1630350000 -0.3773820000
 C -0.2989670000 1.4144300000 -0.5518860000
 C -1.1873990000 2.4565310000 -0.8700810000

C -3.7786080000 -1.9092300000 0.2546080000
C -2.4535710000 -1.4844250000 0.0582790000
C -4.0169830000 -3.2031150000 0.7325630000
C -2.9299510000 -4.0436230000 1.0068230000
C -1.6384950000 -3.5599890000 0.7722190000
N -1.4060170000 -2.3176590000 0.3081700000
C 1.2213360000 1.6392230000 -0.3034910000
C 1.5115170000 3.1526840000 -0.2617180000
C 2.0635280000 0.9673360000 -1.4202120000
C 1.5861040000 0.9878930000 1.0647070000
N 1.4530600000 -0.3569530000 1.1908910000
C 1.7410380000 -0.9635250000 2.3626050000
C 2.1838960000 -0.2590150000 3.4841140000
C 2.3315340000 1.1267000000 3.3718810000
C 2.0306720000 1.7541490000 2.1550480000
C 2.9405440000 1.7016460000 -2.2386800000
C 3.7090930000 1.0378230000 -3.2028920000
C 3.5964080000 -0.3508550000 -3.3306520000
C 2.7028010000 -1.0154990000 -2.4895730000
N 1.9506070000 -0.3726840000 -1.5695370000
H -3.2606420000 2.9752650000 -1.2222630000
H -5.0430940000 -3.5476530000 0.8924050000
H -3.0725930000 -5.0585730000 1.3874960000
H -0.7562540000 -4.1826110000 0.9552590000
H 0.8972530000 3.6444610000 0.5075780000
H 2.5714350000 3.3414830000 -0.0339740000
H 1.2815890000 3.6206620000 -1.2303490000
H 1.6165060000 -2.0512550000 2.3866620000
H 2.4068730000 -0.7906000000 4.4131780000
H 2.6784850000 1.7240320000 4.2208480000
H 2.1444130000 2.8351070000 2.0703120000
H 3.0355910000 2.7824530000 -2.1317950000
H 4.3941090000 1.6059850000 -3.8400560000
H 4.1850480000 -0.9129640000 -4.0608770000
H 2.5749670000 -2.1025560000 -2.5357480000
Fe 0.5147480000 -1.5407750000 -0.3908030000
H -0.8311440000 3.4731480000 -1.0390270000
N 1.6994360000 -3.1615510000 -0.2246300000
H 1.3515410000 -4.1049350000 -0.4387920000
N -0.3129890000 -2.2075040000 -2.3629880000
H -1.2787790000 -1.9007950000 -2.5380590000
H -0.3291850000 -3.2307410000 -2.4636320000
H 0.2289650000 -1.8611660000 -3.1640020000
N 2.9245650000 -3.2850150000 0.3627900000
H -4.6150900000 -1.2377440000 0.0482790000
H -4.1002660000 0.6799740000 -0.6924290000

H 3.4727720000 -4.1016190000 0.0722140000
H 3.4725660000 -2.4203180000 0.3370670000

[(bpyPy₂Me)Fe(MeCN)(NH₂)]²⁺, multiplicity = 2

C -2.5765020000 2.2143490000 -0.9239790000
C -3.0272850000 0.9114830000 -0.6848210000
C -2.0747130000 -0.0931660000 -0.4723320000
N -0.7465140000 0.1920660000 -0.5625180000
C -0.2958820000 1.4578790000 -0.6403340000
C -1.2063690000 2.5047410000 -0.8539930000
C -3.6005400000 -2.0093520000 0.2209930000
C -2.3296420000 -1.4630680000 -0.0070510000
C -3.7031990000 -3.2882290000 0.7789080000
C -2.5294630000 -3.9841920000 1.0964710000
C -1.2914360000 -3.3920280000 0.8267720000
N -1.1841750000 -2.1596540000 0.2871930000
C 1.2062370000 1.6416090000 -0.3426020000
C 1.5566080000 3.1375310000 -0.2868280000
C 2.0616200000 0.9063290000 -1.3913180000
C 1.4633520000 0.9509200000 1.0271770000
N 1.1349990000 -0.3643280000 1.1359600000
C 1.3071990000 -1.0076150000 2.3131890000
C 1.8372850000 -0.3767980000 3.4383580000
C 2.1983040000 0.9705930000 3.3382310000
C 2.0041610000 1.6390160000 2.1230250000
C 3.0270990000 1.5600930000 -2.1718940000
C 3.8012470000 0.8286430000 -3.0796980000
C 3.5955360000 -0.5507650000 -3.1842410000
C 2.6184590000 -1.1417750000 -2.3848040000
N 1.8623420000 -0.4308860000 -1.5107760000
H -3.2950480000 3.0175670000 -1.1107340000
H -4.6854960000 -3.7323070000 0.9638860000
H -2.5591800000 -4.9828550000 1.5401880000
H -0.3574310000 -3.9176230000 1.0376050000
H 0.9525730000 3.6478360000 0.4786860000
H 2.6195350000 3.2833260000 -0.0435810000
H 1.3571660000 3.6151170000 -1.2582350000
H 1.0079840000 -2.0582050000 2.3424880000
H 1.9579020000 -0.9399360000 4.3674760000
H 2.6213400000 1.5040210000 4.1947840000
H 2.2744800000 2.6918500000 2.0358860000
H 3.1784360000 2.6355730000 -2.0751150000
H 4.5545360000 1.3341120000 -3.6914380000
H 4.1765070000 -1.1709880000 -3.8720070000
H 2.4157260000 -2.2138390000 -2.4371040000

Fe 0.4301380000 -1.3244030000 -0.4859370000
 H -0.8600670000 3.5343360000 -0.9512070000
 N 1.5928580000 -2.8115780000 -0.1073600000
 N -0.1713130000 -2.0192930000 -2.0757130000
 H -1.0336820000 -2.5639780000 -2.1900920000
 H 0.2025620000 -1.7475660000 -2.9919590000
 H -4.4960880000 -1.4366110000 -0.0317930000
 H -4.0952360000 0.6863730000 -0.6384280000
 C 2.3266920000 -3.6913760000 0.1045080000
 C 3.2375390000 -4.7935490000 0.3632680000
 H 3.2654340000 -5.0016800000 1.4457980000
 H 4.2486520000 -4.5254470000 0.0142850000
 H 2.8879620000 -5.6907040000 -0.1742790000

[(bpyPy₂Me)Fe(MeCN)(NH₂)]²⁺, multiplicity = 4

C -2.5867440000 2.2428960000 -0.9736560000
 C -3.0517180000 0.9541650000 -0.6832550000
 C -2.1025730000 -0.0434520000 -0.4124210000
 N -0.7855650000 0.2437310000 -0.4650600000
 C -0.3206840000 1.4886340000 -0.6254850000
 C -1.2148100000 2.5334470000 -0.9147810000
 C -3.6762830000 -1.9204380000 0.2785700000
 C -2.3846660000 -1.4228490000 0.0473040000
 C -3.8292830000 -3.2139560000 0.7905500000
 C -2.6867830000 -3.9780380000 1.0594120000
 C -1.4288460000 -3.4269570000 0.7909040000
 N -1.2784530000 -2.1806650000 0.3025850000
 C 1.1951350000 1.6597880000 -0.3419180000
 C 1.5403780000 3.1590220000 -0.2865290000
 C 2.0532900000 0.9441840000 -1.4115540000
 C 1.4704590000 0.9742670000 1.0292470000
 N 1.2110180000 -0.3570950000 1.1512220000
 C 1.3904550000 -0.9763380000 2.3401420000
 C 1.8581170000 -0.3066400000 3.4707640000
 C 2.1502920000 1.0556030000 3.3594070000
 C 1.9503070000 1.6981570000 2.1308670000
 C 2.9714800000 1.6316190000 -2.2211020000
 C 3.7714920000 0.9224950000 -3.1254800000
 C 3.6409570000 -0.4677720000 -3.2122570000
 C 2.6921970000 -1.0918930000 -2.4044290000
 N 1.9217980000 -0.4009810000 -1.5306370000
 H -3.2996580000 3.0393440000 -1.2067990000
 H -4.8290910000 -3.6167940000 0.9772040000
 H -2.7572040000 -4.9911500000 1.4642390000
 H -0.5115880000 -3.9968150000 0.9652380000

H 0.9299320000 3.6667580000 0.4755050000
 H 2.6025550000 3.3132220000 -0.0445780000
 H 1.3365250000 3.6360640000 -1.2570510000
 H 1.1529240000 -2.0427150000 2.3718820000
 H 1.9876600000 -0.8520380000 4.4091800000
 H 2.5259630000 1.6219610000 4.2169470000
 H 2.1681330000 2.7624890000 2.0405550000
 H 3.0723260000 2.7146980000 -2.1491940000
 H 4.4916240000 1.4577080000 -3.7519200000
 H 4.2509770000 -1.0641520000 -3.8956650000
 H 2.5198580000 -2.1712290000 -2.4463300000
 Fe 0.5299200000 -1.4051550000 -0.4577380000
 H -0.8657620000 3.5541500000 -1.0775740000
 N 1.7293690000 -3.0723950000 0.1497200000
 N -0.0335300000 -2.1737980000 -2.0218030000
 H -0.9022530000 -2.7154610000 -2.0847070000
 H 0.1646730000 -1.7327470000 -2.9278700000
 H -4.5509490000 -1.3009650000 0.0665170000
 H -4.1229470000 0.7417780000 -0.6544210000
 C 2.4771270000 -3.9638910000 0.2223490000
 C 3.4050760000 -5.0772900000 0.3128030000
 H 3.5599540000 -5.3418160000 1.3718830000
 H 4.3683450000 -4.7853360000 -0.1378560000
 H 2.9922810000 -5.9437930000 -0.2299620000

[(bpyPy₂Me)Fe(MeCN)(NH₂)]²⁺, multiplicity = 6

C -2.5906420000 2.1900580000 -0.9586400000
 C -3.0497220000 0.9026020000 -0.6629910000
 C -2.1030000000 -0.0876860000 -0.3638940000
 N -0.7774470000 0.1945180000 -0.3841120000
 C -0.3212330000 1.4465420000 -0.5639920000
 C -1.2224410000 2.4790960000 -0.8826080000
 C -3.7521210000 -1.9401170000 0.2025530000
 C -2.4379520000 -1.4676820000 0.0618210000
 C -3.9636580000 -3.2433390000 0.6690660000
 C -2.8595830000 -4.0438550000 0.9872220000
 C -1.5767650000 -3.5128620000 0.8127000000
 N -1.3719150000 -2.2598960000 0.3640950000
 C 1.1928510000 1.6918780000 -0.3119400000
 C 1.4643520000 3.2084490000 -0.2740650000
 C 2.0596180000 1.0244840000 -1.4077890000
 C 1.5610830000 1.0420130000 1.0557780000
 N 1.4222140000 -0.3015020000 1.1817330000
 C 1.7182730000 -0.9029000000 2.3531750000
 C 2.1754970000 -0.1988340000 3.4689850000

C 2.3322620000 1.1850200000 3.3528170000
 C 2.0224210000 1.8099220000 2.1373430000
 C 2.9788980000 1.7482320000 -2.1862430000
 C 3.7798180000 1.0757490000 -3.1177970000
 C 3.6534830000 -0.3103950000 -3.2575980000
 C 2.7096280000 -0.9660360000 -2.4666750000
 N 1.9339580000 -0.3120640000 -1.5735010000
 H -3.3016970000 2.9809880000 -1.2146250000
 H -4.9823460000 -3.6255970000 0.7834840000
 H -2.9797280000 -5.0642750000 1.3606090000
 H -0.6834260000 -4.1046150000 1.0343730000
 H 0.8373320000 3.6959100000 0.4876900000
 H 2.5193380000 3.4109080000 -0.0370610000
 H 1.2396920000 3.6677960000 -1.2482050000
 H 1.5831820000 -1.9881950000 2.3899950000
 H 2.4022880000 -0.7311640000 4.3966010000
 H 2.6920280000 1.7822270000 4.1964000000
 H 2.1424000000 2.8895750000 2.0462170000
 H 3.0817030000 2.8274720000 -2.0715130000
 H 4.4983460000 1.6364790000 -3.7236810000
 H 4.2632440000 -0.8779420000 -3.9656240000
 H 2.5506690000 -2.0464670000 -2.5444080000
 Fe 0.5145860000 -1.5121740000 -0.4407300000
 H -0.8746390000 3.4971380000 -1.0593150000
 N 1.6674490000 -3.1783270000 0.1673340000
 N -0.0484320000 -2.2365590000 -2.1400950000
 H -0.7135310000 -3.0143920000 -2.2405550000
 H 0.1966130000 -1.9072680000 -3.0820590000
 H -4.6018260000 -1.2999630000 -0.0451050000
 H -4.1192090000 0.6813450000 -0.6586400000
 C 2.3698880000 -4.0998380000 0.2944780000
 C 3.2424690000 -5.2476460000 0.4517300000
 H 3.3365630000 -5.4924820000 1.5226840000
 H 4.2361700000 -5.0053700000 0.0391250000
 H 2.8162080000 -6.1073930000 -0.0915820000

[(bpyPy₂Me)Fe(NH₂)(NH₂)]²⁺, multiplicity = 3

C -2.5791080000 2.2326740000 -0.9067130000
 C -3.0495650000 0.9367380000 -0.6626990000
 C -2.1102590000 -0.0808380000 -0.4543720000
 N -0.7811760000 0.1871580000 -0.5469830000
 C -0.3120270000 1.4424360000 -0.6287040000
 C -1.2048010000 2.5044720000 -0.8444330000
 C -3.6592740000 -1.9726580000 0.2642710000
 C -2.3842220000 -1.4481030000 0.0139400000

C -3.7732700000 -3.2535580000 0.8177440000
 C -2.6088670000 -3.9748660000 1.1092140000
 C -1.3644470000 -3.4048050000 0.8192810000
 N -1.2532220000 -2.1709360000 0.2874280000
 C 1.1954110000 1.5970410000 -0.3313080000
 C 1.5691740000 3.0870850000 -0.2628130000
 C 2.0308280000 0.8621800000 -1.3954620000
 C 1.4467440000 0.8896620000 1.0327250000
 N 1.1173080000 -0.4261270000 1.1354070000
 C 1.2724920000 -1.0735480000 2.3123750000
 C 1.7911150000 -0.4472830000 3.4457640000
 C 2.1576210000 0.8982700000 3.3518060000
 C 1.9788300000 1.5712820000 2.1363470000
 C 3.0028750000 1.5127220000 -2.1721880000
 C 3.7606430000 0.7832770000 -3.0941360000
 C 3.5352480000 -0.5918580000 -3.2197080000
 C 2.5552060000 -1.1814330000 -2.4245300000
 N 1.8155360000 -0.4690120000 -1.5379780000
 H -3.2866130000 3.0461580000 -1.0910400000
 H -4.7600910000 -3.6789500000 1.0208630000
 H -2.6499520000 -4.9743120000 1.5489280000
 H -0.4248700000 -3.9332480000 1.0016300000
 H 0.9723090000 3.5999400000 0.5060070000
 H 2.6337920000 3.2145070000 -0.0170470000
 H 1.3774090000 3.5763170000 -1.2299330000
 H 0.9716480000 -2.1245360000 2.3299330000
 H 1.9002210000 -1.0128220000 4.3748820000
 H 2.5736060000 1.4283420000 4.2138270000
 H 2.2547380000 2.6230850000 2.0573750000
 H 3.1733990000 2.5833000000 -2.0562650000
 H 4.5206500000 1.2870450000 -3.6990350000
 H 4.1068170000 -1.2101080000 -3.9170790000
 H 2.3395650000 -2.2504650000 -2.4791130000
 Fe 0.4051680000 -1.3912480000 -0.4887520000
 H -0.8447100000 3.5285570000 -0.9468920000
 N 1.4663140000 -2.8256860000 -0.0906540000
 H 1.5040800000 -3.6638040000 -0.6795310000
 H 2.3096720000 -2.7456660000 0.4894330000
 N -0.2086520000 -2.1162880000 -2.0525070000
 H 0.0373620000 -1.7582750000 -2.9823900000
 H -0.9260070000 -2.8471920000 -2.1187870000
 H -4.5492590000 -1.3830900000 0.0323490000
 H -4.1207520000 0.7286160000 -0.6101900000

[(bpyPy₂Me)Fe(NH₂)(NH₂)]²⁺, multiplicity = 1

C -2.5664860000 2.1928300000 -0.8183330000
C -3.0302110000 0.9036940000 -0.5347420000
C -2.0868690000 -0.1189150000 -0.3644780000
N -0.7646350000 0.1466710000 -0.5028520000
C -0.2903600000 1.3965290000 -0.6401520000
C -1.1891680000 2.4564800000 -0.8361760000
C -3.6363420000 -2.0072030000 0.3250190000
C -2.3572830000 -1.5042380000 0.0470500000
C -3.7702180000 -3.3208220000 0.7852600000
C -2.6175740000 -4.0979920000 0.9495700000
C -1.3730370000 -3.5416320000 0.6385490000
N -1.2322280000 -2.2732960000 0.2039560000
C 1.2244490000 1.5590440000 -0.3877290000
C 1.6004710000 3.0493670000 -0.3569770000
C 2.0723170000 0.7926800000 -1.4227590000
C 1.4611030000 0.8856920000 0.9898780000
N 1.0791880000 -0.4095500000 1.1160030000
C 1.1791600000 -1.0321650000 2.3117530000
C 1.6912740000 -0.3922730000 3.4404010000
C 2.1268590000 0.9307400000 3.3190140000
C 2.0062500000 1.5755170000 2.0824100000
C 3.0480200000 1.4198130000 -2.2118640000
C 3.8268690000 0.6605550000 -3.0934650000
C 3.6185750000 -0.7203170000 -3.1688740000
C 2.6300630000 -1.2881190000 -2.3661910000
N 1.8764380000 -0.5470090000 -1.5154660000
H -3.2781840000 3.0073400000 -0.9803770000
H -4.7593400000 -3.7292040000 1.0104090000
H -2.6669860000 -5.1295310000 1.3063020000
H -0.4674940000 -4.1435850000 0.7376360000
H 1.0120310000 3.5801860000 0.4060140000
H 2.6675900000 3.1798360000 -0.1233880000
H 1.4009310000 3.5165730000 -1.3335160000
H 0.8450010000 -2.0706180000 2.3515500000
H 1.7498740000 -0.9357170000 4.3871800000
H 2.5491650000 1.4640110000 4.1758480000
H 2.3288400000 2.6116000000 1.9758740000
H 3.2055120000 2.4962690000 -2.1392900000
H 4.5885650000 1.1490500000 -3.7087290000
H 4.2044490000 -1.3578180000 -3.8364250000
H 2.4123590000 -2.3598470000 -2.3849780000
Fe 0.4169210000 -1.4345620000 -0.5512190000
H -0.8281510000 3.4749500000 -0.9822380000
N 1.5260840000 -2.7445890000 -0.0479770000
H 1.2461280000 -3.5521530000 0.5193690000
H 2.5267480000 -2.5582000000 0.0921360000

N -0.2621560000 -1.8381460000 -2.1557200000
H -1.2330640000 -2.1394890000 -2.3002040000
H 0.1360120000 -1.4612550000 -3.0232590000
H -4.5148840000 -1.3730260000 0.1859440000
H -4.0989460000 0.7001550000 -0.4376240000

[(bpyPy₂Me)Fe(NH₂)(NH₂)]²⁺, multiplicity = 5

C -2.5489870000 2.1628630000 -0.9993200000
C -3.0382900000 0.8892360000 -0.6925810000
C -2.1223310000 -0.1259330000 -0.3879190000
N -0.7852740000 0.1239680000 -0.4254750000
C -0.2994090000 1.3701080000 -0.5893930000
C -1.1758700000 2.4203370000 -0.9127730000
C -3.8179200000 -1.9471460000 0.1647900000
C -2.4976970000 -1.4778160000 0.0857720000
C -4.0497350000 -3.2239440000 0.6931760000
C -2.9649120000 -3.9970060000 1.1267030000
C -1.6739260000 -3.4677260000 1.0042140000
N -1.4529290000 -2.2404110000 0.5029540000
C 1.2101850000 1.5863590000 -0.3076220000
C 1.5068670000 3.0944370000 -0.2076520000
C 2.0691370000 0.9425480000 -1.4220740000
C 1.5399670000 0.8773640000 1.0367610000
N 1.2574390000 -0.4478310000 1.1687860000
C 1.4830080000 -1.0885400000 2.3396750000
C 2.0303410000 -0.4423650000 3.4467590000
C 2.3576440000 0.9106630000 3.3256700000
C 2.1075120000 1.5709540000 2.1160610000
C 2.9906010000 1.6675470000 -2.1959170000
C 3.7528150000 0.9933460000 -3.1587210000
C 3.5868810000 -0.3868510000 -3.3225250000
C 2.6526610000 -1.0400380000 -2.5160640000
N 1.9112290000 -0.3832440000 -1.5999480000
H -3.2401510000 2.9692550000 -1.2604630000
H -5.0711280000 -3.6101160000 0.7616420000
H -3.1070440000 -4.9964000000 1.5456920000
H -0.7874980000 -4.0357470000 1.3043120000
H 0.8938640000 3.5621380000 0.5773590000
H 2.5673190000 3.2672950000 0.0268770000
H 1.2877110000 3.5938230000 -1.1630300000
H 1.2110450000 -2.1474030000 2.3756640000
H 2.1936320000 -0.9988060000 4.3731980000
H 2.7988100000 1.4579970000 4.1640890000
H 2.3560940000 2.6279300000 2.0225620000
H 3.1226440000 2.7410720000 -2.0555650000

H 4.4738830000 1.5469180000 -3.7683270000
 H 4.1681090000 -0.9537460000 -4.0550220000
 H 2.4849000000 -2.1190380000 -2.5922790000
 Fe 0.4360150000 -1.5042190000 -0.3666030000
 H -0.8004210000 3.4288950000 -1.0847320000
 N 1.5244440000 -2.9354710000 -0.0144550000
 H 1.6055730000 -3.7417390000 -0.6403440000
 H 2.3524580000 -2.8564010000 0.5876060000
 N -0.1917640000 -2.2312640000 -1.9429090000
 H 0.1499290000 -1.9771940000 -2.8764010000
 H -0.7674970000 -3.0806550000 -1.9798430000
 H -4.6523530000 -1.3329930000 -0.1814320000
 H -4.1129450000 0.6951440000 -0.6706440000

[(bpyPy₂Me)Fe(NH)(NH₃)]²⁺, multiplicity = 3

C -2.5865660000 2.2469210000 -0.8995420000
 C -3.0541710000 0.9510590000 -0.6527740000
 C -2.1116290000 -0.0673940000 -0.4544460000
 N -0.7821740000 0.1981150000 -0.5663570000
 C -0.3176970000 1.4562660000 -0.6471530000
 C -1.2107730000 2.5193430000 -0.8483770000
 C -3.6569860000 -1.9608530000 0.2775790000
 C -2.3830390000 -1.4352800000 0.0191860000
 C -3.7660780000 -3.2433920000 0.8272820000
 C -2.5988210000 -3.9688200000 1.1006440000
 C -1.3578510000 -3.3981610000 0.8009930000
 N -1.2495760000 -2.1597200000 0.2772550000
 C 1.1893250000 1.6024640000 -0.3463730000
 C 1.5711830000 3.0900690000 -0.2752100000
 C 2.0346990000 0.8610150000 -1.3990330000
 C 1.4284650000 0.8908530000 1.0187090000
 N 1.1034620000 -0.4279400000 1.1199440000
 C 1.2719240000 -1.0821030000 2.2920120000
 C 1.7850390000 -0.4551750000 3.4267550000
 C 2.1392420000 0.8946280000 3.3398360000
 C 1.9564920000 1.5696190000 2.1269850000
 C 2.9960520000 1.5104240000 -2.1900630000
 C 3.7793860000 0.7715530000 -3.0830210000
 C 3.5967530000 -0.6138670000 -3.1579130000
 C 2.6245390000 -1.2011790000 -2.3511620000
 N 1.8485420000 -0.4785510000 -1.5041390000
 H -3.2960950000 3.0607460000 -1.0745550000
 H -4.7510560000 -3.6687680000 1.0393030000
 H -2.6375650000 -4.9718540000 1.5324960000
 H -0.4146260000 -3.9289490000 0.9605580000

H 0.9764110000 3.6051460000 0.4937420000
 H 2.6367110000 3.2121830000 -0.0299630000
 H 1.3799560000 3.5811270000 -1.2416090000
 H 0.9895630000 -2.1376630000 2.2981970000
 H 1.9040380000 -1.0259610000 4.3514990000
 H 2.5524890000 1.4239160000 4.2036150000
 H 2.2270430000 2.6230350000 2.0500470000
 H 3.1394740000 2.5882310000 -2.1068850000
 H 4.5292650000 1.2751770000 -3.7006150000
 H 4.1963420000 -1.2409490000 -3.8232750000
 H 2.4508530000 -2.2810290000 -2.3530630000
 Fe 0.4165210000 -1.3793910000 -0.4797790000
 H -0.8520090000 3.5442750000 -0.9482810000
 N 1.4143690000 -2.7644200000 -0.1769490000
 H 2.3329490000 -2.9275020000 0.2668180000
 N -0.3116590000 -2.0946750000 -2.2324470000
 H -1.2205630000 -1.6966010000 -2.5043740000
 H -0.4390980000 -3.1130320000 -2.1808520000
 H 0.3142730000 -1.9204610000 -3.0289600000
 H -4.5491000000 -1.3707620000 0.0552150000
 H -4.1248150000 0.7437340000 -0.5867010000

[(bpyPy₂Me)Fe(NH)(NH₃)]²⁺, multiplicity = 1

C -2.5980530000 2.2382830000 -0.8837030000
 C -3.0712430000 0.9490750000 -0.6114400000
 C -2.1294680000 -0.0684800000 -0.4044030000
 N -0.8034580000 0.1932800000 -0.5153670000
 C -0.3310090000 1.4440940000 -0.6379090000
 C -1.2203160000 2.5068800000 -0.8583630000
 C -3.6731890000 -1.9618600000 0.3201280000
 C -2.3984710000 -1.4440200000 0.0495570000
 C -3.7870990000 -3.2577040000 0.8366220000
 C -2.6226800000 -4.0034340000 1.0614940000
 C -1.3819790000 -3.4385630000 0.7478710000
 N -1.2686510000 -2.1867030000 0.2613440000
 C 1.1821750000 1.5921640000 -0.3581800000
 C 1.5619470000 3.0816430000 -0.3073740000
 C 2.0405330000 0.8364090000 -1.3927750000
 C 1.4349620000 0.8970900000 1.0090690000
 N 1.1304390000 -0.4253960000 1.1126110000
 C 1.3149180000 -1.0746940000 2.2873610000
 C 1.8234980000 -0.4365000000 3.4173960000
 C 2.1527990000 0.9193600000 3.3273130000
 C 1.9547740000 1.5877800000 2.1132890000
 C 2.9986060000 1.4810640000 -2.1905070000

C 3.8061830000 0.7342910000 -3.0554000000
 C 3.6506960000 -0.6555260000 -3.0966410000
 C 2.6781740000 -1.2388940000 -2.2876650000
 N 1.8802320000 -0.5105260000 -1.4645020000
 H -3.3056780000 3.0519900000 -1.0672780000
 H -4.7723720000 -3.6764970000 1.0602900000
 H -2.6635910000 -5.0169690000 1.4682360000
 H -0.4376030000 -3.9806900000 0.8603500000
 H 0.9666250000 3.6055970000 0.4551190000
 H 2.6274350000 3.2093690000 -0.0647400000
 H 1.3683760000 3.5602910000 -1.2795310000
 H 1.0442220000 -2.1338850000 2.3009180000
 H 1.9582700000 -1.0042400000 4.3418290000
 H 2.5591080000 1.4574640000 4.1888620000
 H 2.2053520000 2.6458430000 2.0318360000
 H 3.1202740000 2.5633470000 -2.1360130000
 H 4.5527090000 1.2361820000 -3.6783520000
 H 4.2685700000 -1.2883920000 -3.7392710000
 H 2.5184430000 -2.3214410000 -2.2862600000
 Fe 0.4293030000 -1.3901060000 -0.4699790000
 H -0.8602990000 3.5273430000 -0.9929850000
 N 1.2909790000 -2.8207760000 -0.1097560000
 H 2.3076000000 -2.6235140000 0.0613720000
 N -0.3129240000 -2.0364620000 -2.2405220000
 H -1.1151030000 -1.4846510000 -2.5717700000
 H -0.6315500000 -3.0098810000 -2.1657110000
 H 0.3761020000 -2.0166940000 -3.0039550000
 H -4.5623430000 -1.3549210000 0.1340020000
 H -4.1428170000 0.7480280000 -0.5417200000

[(bpyPy₂Me)Fe(NH)(NH₃)]²⁺, multiplicity = 5

C -2.5930951701 2.2388102740 -0.9773191524
 C -3.0677731407 0.9530798313 -0.6822881912
 C -2.1227450836 -0.0406559036 -0.3838112707
 N -0.8040995458 0.2377912160 -0.4146641419
 C -0.3377154715 1.4755608051 -0.5970483039
 C -1.2193767911 2.5241466153 -0.9095010533
 C -3.6871798171 -1.9079161949 0.3641042371
 C -2.4043089947 -1.4202573574 0.0767687082
 C -3.8295888488 -3.2048053805 0.8725372179
 C -2.6873252078 -3.9888881655 1.0786624377
 C -1.4376045345 -3.4545594845 0.7509950529
 N -1.2994528175 -2.2027664591 0.2684675855
 C 1.1816764393 1.6238700173 -0.3151283269
 C 1.5593289376 3.1146542184 -0.2660565566

C 2.0149655886 0.8801112875 -1.3846266202
 C 1.4580807635 0.9332102262 1.0499534062
 N 1.2877731739 -0.4125087928 1.1319741920
 C 1.5255600002 -1.0738383092 2.2844253691
 C 1.9330546914 -0.4124000391 3.4439957586
 C 2.1122521078 0.9732740422 3.3864084333
 C 1.8787454890 1.6489660588 2.1804599048
 C 2.9155259829 1.5514746860 -2.2277245679
 C 3.7221903654 0.8286279490 -3.1142311073
 C 3.6366155382 -0.5678685300 -3.1322131985
 C 2.7202050628 -1.1837972132 -2.2827360090
 N 1.9150242683 -0.4736183412 -1.4550657102
 H -3.2997339207 3.0355896964 -1.2273839000
 H -4.8241254846 -3.5956243215 1.1064341165
 H -2.7530048758 -5.0046663534 1.4757349012
 H -0.5108129966 -4.0259505075 0.8555187786
 H 0.9583104544 3.6365242336 0.4934435523
 H 2.6242671413 3.2458570512 -0.0210670739
 H 1.3636316695 3.5955449190 -1.2362832577
 H 1.3929676338 -2.1598944406 2.2450991661
 H 2.1169075140 -0.9815150905 4.3591602939
 H 2.4406719822 1.5318162269 4.2681870624
 H 2.0274566149 2.7284471878 2.1294070602
 H 2.9962110982 2.6382315506 -2.1885939304
 H 4.4225607888 1.3567673078 -3.7686647103
 H 4.2665304314 -1.1794529014 -3.7836943350
 H 2.6082970167 -2.2714142799 -2.2299891341
 Fe 0.5016690633 -1.4738120049 -0.4513344025
 H -0.8640986809 3.5410789059 -1.0817572610
 N 1.4543920528 -3.0214115593 -0.1788123534
 H 1.9594999684 -3.8725628600 0.1192186503
 N -0.2570334438 -2.0619226160 -2.2754336082
 H -0.9602226754 -1.4187596753 -2.6627960746
 H -0.6955192786 -2.9871642757 -2.1960562468
 H 0.4770127714 -2.1569777517 -2.9887719650
 H -4.5631640074 -1.2752736239 0.2022575796
 H -4.1399908229 0.7422941264 -0.6753620013

[(bpyPy₂Me)Fe(NH₃)(NH)]²⁺, multiplicity = 3

C -2.5396260000 2.1898430000 -0.9808880000
 C -3.0121980000 0.8945440000 -0.7409470000
 C -2.0750150000 -0.1206580000 -0.5085400000
 N -0.7442430000 0.1469790000 -0.5902160000
 C -0.2735420000 1.4069910000 -0.6521990000
 C -1.1672220000 2.4644260000 -0.8832480000

C -3.6371290000 -1.9783890000 0.2485790000
C -2.3540910000 -1.4706920000 0.0034720000
C -3.7733670000 -3.2232710000 0.8732080000
C -2.6201240000 -3.9238280000 1.2449910000
C -1.3684560000 -3.3706890000 0.9537600000
N -1.2285430000 -2.1780640000 0.3445380000
C 1.2262500000 1.5767900000 -0.3126720000
C 1.5831220000 3.0709110000 -0.2422960000
C 2.0902910000 0.8481690000 -1.3592940000
C 1.4490350000 0.8814400000 1.0601980000
N 1.1200270000 -0.4343710000 1.1580440000
C 1.2575870000 -1.0761920000 2.3398320000
C 1.7527760000 -0.4475640000 3.4822220000
C 2.1175340000 0.8990000000 3.3916650000
C 1.9601730000 1.5678570000 2.1712330000
C 3.0841980000 1.5022820000 -2.1045650000
C 3.8167370000 0.7927800000 -3.0622550000
C 3.5254500000 -0.5594850000 -3.2704410000
C 2.5280340000 -1.1508960000 -2.4981730000
N 1.8423610000 -0.4715480000 -1.5470960000
H -3.2440170000 3.0015890000 -1.1836720000
H -4.7669550000 -3.6352820000 1.0706820000
H -2.6732170000 -4.8938350000 1.7449530000
H -0.4565070000 -3.9133250000 1.2134490000
H 0.9620210000 3.5819260000 0.5084090000
H 2.6397020000 3.2095820000 0.0303780000
H 1.4125460000 3.5532310000 -1.2168440000
H 0.9570060000 -2.1272820000 2.3672030000
H 1.8456860000 -1.0108890000 4.4144380000
H 2.5160560000 1.4320650000 4.2600350000
H 2.2351720000 2.6200860000 2.0939510000
H 3.2853220000 2.5613600000 -1.9428540000
H 4.5941610000 1.2977290000 -3.6433950000
H 4.0512450000 -1.1560620000 -4.0206960000
H 2.2368880000 -2.1924570000 -2.6533940000
Fe 0.4105400000 -1.3929590000 -0.5085760000
H -0.8083910000 3.4902080000 -0.9729750000
N 1.6902740000 -2.9126160000 -0.1210920000
H 2.5114050000 -2.5954320000 0.4102220000
N -0.1613440000 -2.1984370000 -1.9466760000
H -0.4498750000 -3.1727910000 -2.1410500000
H -4.5181500000 -1.4009830000 -0.0413080000
H -4.0839560000 0.6855490000 -0.7045300000
H 1.2955670000 -3.6984520000 0.4104930000
H 2.0566400000 -3.3407320000 -0.9801060000

[(bpyPy₂Me)Fe(NH₃)(NH)]²⁺, multiplicity = 1

C -2.5545170000 2.1810540000 -0.8727090000
C -3.0225240000 0.8863680000 -0.6268440000
C -2.0820850000 -0.1347450000 -0.4395700000
N -0.7517290000 0.1304610000 -0.5542460000
C -0.2763400000 1.3900410000 -0.6375870000
C -1.1780930000 2.4479380000 -0.8307000000
C -3.6266020000 -2.0202510000 0.2853790000
C -2.3513800000 -1.5057650000 0.0108590000
C -3.7426830000 -3.3082070000 0.8175850000
C -2.5779720000 -4.0475370000 1.0615960000
C -1.3367340000 -3.4844710000 0.7506150000
N -1.2140290000 -2.2401020000 0.2411040000
C 1.2311660000 1.5717040000 -0.3444950000
C 1.5820000000 3.0684400000 -0.3020150000
C 2.0975860000 0.8288650000 -1.3788590000
C 1.4683480000 0.9007700000 1.0378080000
N 1.1110570000 -0.4025440000 1.1564510000
C 1.2094160000 -1.0143520000 2.3558990000
C 1.7169980000 -0.3755860000 3.4878010000
C 2.1302560000 0.9546440000 3.3679430000
C 1.9940950000 1.6013790000 2.1331060000
C 3.0945200000 1.4731760000 -2.1284430000
C 3.8636720000 0.7398410000 -3.0392590000
C 3.6126850000 -0.6274370000 -3.1916770000
C 2.6008820000 -1.2061730000 -2.4264880000
N 1.8722920000 -0.4986050000 -1.5311330000
H -3.2621160000 2.9973010000 -1.0435500000
H -4.7283940000 -3.7266880000 1.0390820000
H -2.6172640000 -5.0566580000 1.4785010000
H -0.4181680000 -4.0534320000 0.9094550000
H 0.9745170000 3.5878570000 0.4538450000
H 2.6426420000 3.2135910000 -0.0495160000
H 1.3930380000 3.5370290000 -1.2800240000
H 0.8566020000 -2.0482500000 2.4158060000
H 1.7783980000 -0.9174960000 4.4352660000
H 2.5418560000 1.4940640000 4.2261980000
H 2.2946170000 2.6447410000 2.0333500000
H 3.2735540000 2.5414310000 -2.0047140000
H 4.6444100000 1.2376880000 -3.6222660000
H 4.1793430000 -1.2445250000 -3.8942040000
H 2.3319460000 -2.2587000000 -2.5427250000
Fe 0.3927440000 -1.4159150000 -0.5528110000
H -0.8189240000 3.4722580000 -0.9329690000
N 1.6661440000 -2.8973240000 -0.0419790000
H 2.6420610000 -2.6008590000 -0.1753150000

N -0.0540660000 -2.0556460000 -2.0722480000
H -1.0256370000 -2.4484330000 -2.0708060000
H -4.5147400000 -1.4153010000 0.0886370000
H -4.0927120000 0.6772430000 -0.5606380000
H 1.6075640000 -3.2015170000 0.9379860000
H 1.5401370000 -3.7432100000 -0.6105240000

[(bpyPy₂Me)Fe(NH₃)(NH)]²⁺, multiplicity = 5

C -2.5125240000 2.1726860000 -1.0370240000
C -2.9992830000 0.8917110000 -0.7535490000
C -2.0734210000 -0.1180140000 -0.4517050000
N -0.7462850000 0.1407700000 -0.4784600000
C -0.2656360000 1.3880980000 -0.6137190000
C -1.1410170000 2.4417030000 -0.9284780000
C -3.7384530000 -1.9254880000 0.2046410000
C -2.4199090000 -1.4703420000 0.0452460000
C -3.9619110000 -3.1830400000 0.7771930000
C -2.8641800000 -3.9520650000 1.1817540000
C -1.5768520000 -3.4412600000 0.9785420000
N -1.3600860000 -2.2337640000 0.4278350000
C 1.2421640000 1.5807360000 -0.2961860000
C 1.5614860000 3.0837770000 -0.1984590000
C 2.0992260000 0.9195650000 -1.3991500000
C 1.5181470000 0.8700360000 1.0604150000
N 1.2392460000 -0.4574320000 1.1733120000
C 1.3973390000 -1.0842240000 2.3618000000
C 1.8722350000 -0.4329860000 3.4992090000
C 2.1991290000 0.9215700000 3.3931610000
C 2.0153960000 1.5743670000 2.1681730000
C 3.0354770000 1.6285920000 -2.1689170000
C 3.7545950000 0.9585390000 -3.1671480000
C 3.5159420000 -0.4022030000 -3.3900060000
C 2.5675010000 -1.0440440000 -2.5934960000
N 1.8956080000 -0.3976880000 -1.6157660000
H -3.2065410000 2.9779300000 -1.2948130000
H -4.9827470000 -3.5542180000 0.9073760000
H -2.9908060000 -4.9353100000 1.6416300000
H -0.6953480000 -4.0228510000 1.2647900000
H 0.9356400000 3.5653730000 0.5676690000
H 2.6179480000 3.2439420000 0.0622960000
H 1.3694280000 3.5807120000 -1.1611550000
H 1.1273730000 -2.1431980000 2.3987640000
H 1.9813120000 -0.9856190000 4.4359860000
H 2.5862480000 1.4749210000 4.2539530000
H 2.2574650000 2.6338640000 2.0856490000

H 3.2076290000 2.6920100000 -2.0004680000
 H 4.4877480000 1.5040390000 -3.7693500000
 H 4.0437810000 -0.9612620000 -4.1672360000
 H 2.3101160000 -2.0978520000 -2.7363040000
 Fe 0.5365150000 -1.5331530000 -0.4403800000
 H -0.7725180000 3.4570420000 -1.0768500000
 N 1.8506850000 -3.1061960000 0.0445700000
 H 2.7192700000 -2.7798730000 0.4883350000
 N -0.0215190000 -2.4146080000 -1.8135620000
 H -0.4533830000 -3.3487280000 -1.9134360000
 H -4.5802170000 -1.3045590000 -0.1103090000
 H -4.0736250000 0.6940330000 -0.7455070000
 H 1.4614820000 -3.8240500000 0.6695940000
 H 2.1279660000 -3.6138350000 -0.8045110000

[(bpyPy₂Me)Fe(NH₂)(NH₃)]³⁺, multiplicity = 3

C -2.5750700000 2.2362470000 -0.9707640000
 C -3.0472160000 0.9405690000 -0.7237130000
 C -2.1098880000 -0.0704970000 -0.4884120000
 N -0.7777330000 0.1995890000 -0.5692140000
 C -0.3118500000 1.4573580000 -0.6497320000
 C -1.2035330000 2.5138960000 -0.8860840000
 C -3.6565990000 -1.9516170000 0.2563520000
 C -2.3838920000 -1.4280820000 0.0053510000
 C -3.7695230000 -3.2169910000 0.8461260000
 C -2.6071290000 -3.9258780000 1.1739680000
 C -1.3623230000 -3.3670920000 0.8731610000
 N -1.2531550000 -2.1476860000 0.3024820000
 C 1.1873530000 1.6092510000 -0.3288790000
 C 1.5677650000 3.0960940000 -0.2445810000
 C 2.0202160000 0.8779530000 -1.3947690000
 C 1.4313960000 0.8863740000 1.0279070000
 N 1.1333830000 -0.4419880000 1.1181350000
 C 1.3157690000 -1.1227970000 2.2745670000
 C 1.8128440000 -0.5023530000 3.4184340000
 C 2.1374650000 0.8555610000 3.3485900000
 C 1.9459630000 1.5513220000 2.1454420000
 C 2.9712070000 1.5276170000 -2.1925850000
 C 3.7455230000 0.7891200000 -3.0944240000
 C 3.5705970000 -0.5972840000 -3.1674630000
 C 2.6088480000 -1.1892180000 -2.3547940000
 N 1.8349980000 -0.4620590000 -1.5080700000
 H -3.2824350000 3.0458310000 -1.1709210000
 H -4.7570780000 -3.6399100000 1.0506560000
 H -2.6487270000 -4.9089640000 1.6493760000

H -0.4323870000 -3.8976820000 1.0913000000
 H 0.9674310000 3.6033480000 0.5254260000
 H 2.6323590000 3.2141420000 0.0056000000
 H 1.3813000000 3.5927990000 -1.2084300000
 H 1.0607120000 -2.1854340000 2.2637190000
 H 1.9440360000 -1.0845210000 4.3336830000
 H 2.5401100000 1.3796150000 4.2203160000
 H 2.1988600000 2.6101480000 2.0882410000
 H 3.1160170000 2.6047030000 -2.1066370000
 H 4.4884440000 1.2941490000 -3.7186140000
 H 4.1671520000 -1.2232150000 -3.8356750000
 H 2.4497220000 -2.2708390000 -2.3625740000
 Fe 0.4073000000 -1.3524270000 -0.4601050000
 H -0.8442530000 3.5389240000 -0.9840000000
 N 1.4189240000 -2.8596560000 -0.2069750000
 H 1.1783930000 -3.8001080000 -0.5482760000
 H 2.3610330000 -2.8543200000 0.2067300000
 N -0.2974570000 -2.1188030000 -2.1901170000
 H -1.0959930000 -1.5798640000 -2.5538760000
 H -0.6108860000 -3.0947210000 -2.1030400000
 H 0.4039840000 -2.1065580000 -2.9422800000
 H -4.5466210000 -1.3720580000 0.0012380000
 H -4.1182880000 0.7307670000 -0.6852390000

[(bpyPy₂Me)Fe(NH₂)(NH₃)]³⁺, multiplicity = 1

C -2.5600290000 2.1972380000 -0.9935870000
 C -3.0362370000 0.9061110000 -0.7356780000
 C -2.1027030000 -0.0994490000 -0.4671150000
 N -0.7670780000 0.1696240000 -0.5208680000
 C -0.2971490000 1.4278010000 -0.6250110000
 C -1.1881870000 2.4750750000 -0.8956290000
 C -3.6551700000 -1.9685480000 0.2883710000
 C -2.3806360000 -1.4531960000 0.0185340000
 C -3.7713100000 -3.2305230000 0.8810000000
 C -2.6071900000 -3.9419450000 1.1946420000
 C -1.3653430000 -3.3856350000 0.8741190000
 N -1.2482550000 -2.1743570000 0.2941920000
 C 1.1997250000 1.6079930000 -0.3150080000
 C 1.5545830000 3.1071690000 -0.2494010000
 C 2.0491500000 0.8657390000 -1.3616650000
 C 1.4513150000 0.8946160000 1.0420220000
 N 1.1141920000 -0.4153230000 1.1418270000
 C 1.2334180000 -1.0739800000 2.3197120000
 C 1.7390440000 -0.4527470000 3.4605820000
 C 2.1349230000 0.8839300000 3.3711170000

C 1.9868980000 1.5567050000 2.1532560000
 C 3.0117110000 1.5069470000 -2.1547360000
 C 3.7739460000 0.7633400000 -3.0616500000
 C 3.5696730000 -0.6184970000 -3.1506380000
 C 2.6001960000 -1.2000750000 -2.3390530000
 N 1.8533010000 -0.4712490000 -1.4696490000
 H -3.2635060000 3.0035860000 -1.2191220000
 H -4.7578520000 -3.6445350000 1.1068240000
 H -2.6430080000 -4.9179060000 1.6840990000
 H -0.4362150000 -3.9056010000 1.1050700000
 H 0.9425750000 3.6098810000 0.5135980000
 H 2.6158200000 3.2430630000 0.0031670000
 H 1.3621390000 3.5874780000 -1.2203640000
 H 0.9103480000 -2.1168440000 2.3404830000
 H 1.8236750000 -1.0232270000 4.3890260000
 H 2.5496590000 1.4080810000 4.2370250000
 H 2.2861430000 2.5976220000 2.0735640000
 H 3.1664520000 2.5829410000 -2.0673130000
 H 4.5237600000 1.2608320000 -3.6835590000
 H 4.1513320000 -1.2495450000 -3.8275450000
 H 2.4182700000 -2.2779010000 -2.3648890000
 Fe 0.4160580000 -1.3763490000 -0.4412920000
 H -0.8251510000 3.4960500000 -1.0146880000
 N 1.3860630000 -2.7772420000 -0.0961120000
 H 1.0525940000 -3.7568440000 -0.0700990000
 H 2.3892230000 -2.7683700000 0.1635500000
 N -0.3283900000 -2.0596650000 -2.1855260000
 H -1.1166380000 -1.4938540000 -2.5307690000
 H -0.6603870000 -3.0311370000 -2.1239450000
 H 0.3733420000 -2.0449610000 -2.9369180000
 H -4.5434210000 -1.3793130000 0.0504570000
 H -4.1075320000 0.6940420000 -0.7193130000

[(bpyPy₂Me)Fe(NH₂)(NH₃)]³⁺, multiplicity = 5

C -2.5729800000 2.1755620000 -0.9182010000
 C -3.0535180000 0.8895900000 -0.6485670000
 C -2.1295070000 -0.1266100000 -0.3899420000
 N -0.7875490000 0.1393480000 -0.4535670000
 C -0.3047190000 1.3939410000 -0.5827270000
 C -1.1993250000 2.4417590000 -0.8473420000
 C -3.7466830000 -1.9802380000 0.2595120000
 C -2.4538490000 -1.4920460000 0.0425270000
 C -3.9064550000 -3.2793870000 0.7609440000
 C -2.7745640000 -4.0579510000 1.0347050000
 C -1.5083530000 -3.5254450000 0.7775840000

N -1.3572300000 -2.2738570000 0.2951260000
 C 1.2013400000 1.6028680000 -0.3110400000
 C 1.5281340000 3.1062570000 -0.2957490000
 C 2.0465980000 0.8657790000 -1.3721200000
 C 1.5164190000 0.9592580000 1.0709690000
 N 1.2224050000 -0.3543800000 1.2326220000
 C 1.4460230000 -0.9835980000 2.4074630000
 C 2.0015260000 -0.3160970000 3.4992540000
 C 2.3288450000 1.0352220000 3.3514740000
 C 2.0832140000 1.6795320000 2.1297090000
 C 3.0175030000 1.5209050000 -2.1442800000
 C 3.8037560000 0.7873720000 -3.0396650000
 C 3.6155350000 -0.5950950000 -3.1390460000
 C 2.6327600000 -1.1882300000 -2.3501590000
 N 1.8578420000 -0.4693970000 -1.5026040000
 H -3.2731480000 2.9861650000 -1.1382870000
 H -4.9101960000 -3.6761030000 0.9374720000
 H -2.8587790000 -5.0715780000 1.4343670000
 H -0.5943730000 -4.0997390000 0.9525670000
 H 0.9267900000 3.6224050000 0.4675060000
 H 2.5913470000 3.2683220000 -0.0667730000
 H 1.3148990000 3.5584770000 -1.2755760000
 H 1.1686250000 -2.0406240000 2.4675990000
 H 2.1679130000 -0.8537880000 4.4360090000
 H 2.7705180000 1.5958950000 4.1806690000
 H 2.3340910000 2.7342570000 2.0146200000
 H 3.1696580000 2.5956320000 -2.0450130000
 H 4.5622190000 1.2950810000 -3.6428070000
 H 4.2138530000 -1.2151450000 -3.8114300000
 H 2.4552240000 -2.2656590000 -2.3919710000
 Fe 0.3723990000 -1.4366510000 -0.3758730000
 H -0.8345600000 3.4602110000 -0.9803280000
 N 1.3974890000 -2.9240840000 -0.1459380000
 H 1.3575550000 -3.7439020000 -0.7672640000
 H 2.1714240000 -2.9962710000 0.5295180000
 N -0.3829140000 -2.0880200000 -2.3584160000
 H -1.1547500000 -1.4940010000 -2.6902480000
 H -0.7461460000 -3.0504580000 -2.3407670000
 H 0.3229740000 -2.0619840000 -3.1048310000
 H -4.6165910000 -1.3546720000 0.0478300000
 H -4.1256250000 0.6839210000 -0.6229590000

[(bpyPy₂Me)Fe(N)(NH₃)]²⁺, multiplicity = 2

C -2.6071360000 2.2491750000 -0.8674970000
 C -3.0690000000 0.9536270000 -0.6046050000

C -2.1167530000 -0.0589300000 -0.4161430000
N -0.7969130000 0.2154510000 -0.5397050000
C -0.3352590000 1.4680730000 -0.6520380000
C -1.2315680000 2.5297310000 -0.8503920000
C -3.6463400000 -1.9600610000 0.3133500000
C -2.3737460000 -1.4384450000 0.0413150000
C -3.7588270000 -3.2532530000 0.8367570000
C -2.5941460000 -3.9938380000 1.0735590000
C -1.3542320000 -3.4263820000 0.7623180000
N -1.2428440000 -2.1788440000 0.2628070000
C 1.1789030000 1.6074450000 -0.3747010000
C 1.5652280000 3.0950590000 -0.3149670000
C 2.0285490000 0.8573490000 -1.4223980000
C 1.4268460000 0.9050130000 0.9931110000
N 1.1210100000 -0.4171730000 1.1053990000
C 1.3023600000 -1.0673540000 2.2786370000
C 1.8057310000 -0.4263010000 3.4093860000
C 2.1346220000 0.9291220000 3.3160520000
C 1.9417740000 1.5955020000 2.0998420000
C 2.9541760000 1.5152400000 -2.2477540000
C 3.7660130000 0.7771270000 -3.1160640000
C 3.6549420000 -0.6172710000 -3.1297890000
C 2.7115600000 -1.2152110000 -2.2972910000
N 1.9033680000 -0.4931030000 -1.4826850000
H -3.3232720000 3.0590650000 -1.0345590000
H -4.7443500000 -3.6737270000 1.0567140000
H -2.6329800000 -5.0054340000 1.4861480000
H -0.4140270000 -3.9705300000 0.8960940000
H 0.9769200000 3.6142520000 0.4565750000
H 2.6335410000 3.2179570000 -0.0824610000
H 1.3619080000 3.5809730000 -1.2812710000
H 1.0395360000 -2.1279380000 2.2905990000
H 1.9375540000 -0.9924670000 4.3349960000
H 2.5378660000 1.4699700000 4.1773210000
H 2.1909760000 2.6538220000 2.0188070000
H 3.0482590000 2.6007690000 -2.2121220000
H 4.4852340000 1.2899830000 -3.7616210000
H 4.2837440000 -1.2418870000 -3.7695880000
H 2.5883610000 -2.3014700000 -2.2560860000
Fe 0.4636820000 -1.4162630000 -0.4866660000
H -0.8807390000 3.5554050000 -0.9719560000
N 1.3281760000 -2.7375360000 -0.1999760000
N -0.2834020000 -1.9953650000 -2.2638940000
H -0.9545850000 -1.3141590000 -2.6418530000
H -0.7705370000 -2.8980350000 -2.2049180000
H 0.4438150000 -2.1068930000 -2.9822260000

H -4.5369440000 -1.3567990000 0.1222290000
H -4.1386560000 0.7469910000 -0.5251080000

[(bpyPy₂Me)Fe(N)(NH₃)]²⁺, multiplicity = 4

C -2.6148920000 2.2853280000 -0.8877650000
C -3.0828070000 0.9893210000 -0.6353870000
C -2.1355290000 -0.0256510000 -0.4418580000
N -0.8109360000 0.2406500000 -0.5528240000
C -0.3473990000 1.4936670000 -0.6486710000
C -1.2387380000 2.5592600000 -0.8522270000
C -3.6682440000 -1.9316960000 0.2870090000
C -2.3990470000 -1.4019820000 0.0207310000
C -3.7718530000 -3.2225590000 0.8198800000
C -2.6063550000 -3.9604430000 1.0687400000
C -1.3687310000 -3.3927050000 0.7559420000
N -1.2690580000 -2.1432050000 0.2553580000
C 1.1664770000 1.6308000000 -0.3603720000
C 1.5605630000 3.1158040000 -0.2990230000
C 2.0067090000 0.8765640000 -1.4113460000
C 1.4200800000 0.9248610000 1.0049070000
N 1.1727020000 -0.4116170000 1.0891750000
C 1.4075750000 -1.0954780000 2.2313260000
C 1.8789220000 -0.4612090000 3.3805210000
C 2.1341530000 0.9123670000 3.3233590000
C 1.9106250000 1.6066230000 2.1257420000
C 2.9417790000 1.5204680000 -2.2347030000
C 3.7488140000 0.7683140000 -3.0969030000
C 3.6269590000 -0.6255840000 -3.1057220000
C 2.6753150000 -1.2123920000 -2.2751290000
N 1.8695590000 -0.4739780000 -1.4728020000
H -3.3260510000 3.0983650000 -1.0598850000
H -4.7563670000 -3.6477670000 1.0356260000
H -2.6461230000 -4.9703140000 1.4848550000
H -0.4226760000 -3.9302180000 0.8823120000
H 0.9705320000 3.6380560000 0.4691140000
H 2.6281660000 3.2314600000 -0.0590730000
H 1.3657510000 3.6034860000 -1.2662110000
H 1.2215470000 -2.1728650000 2.1927430000
H 2.0510080000 -1.0444990000 4.2886220000
H 2.5158040000 1.4468120000 4.1984440000
H 2.1215070000 2.6750670000 2.0726660000
H 3.0493060000 2.6048960000 -2.2012010000
H 4.4762020000 1.2713050000 -3.7411340000
H 4.2544150000 -1.2574140000 -3.7395650000
H 2.5356150000 -2.2967820000 -2.2203410000

Fe 0.4151040000 -1.3634960000 -0.4673740000
H -0.8821030000 3.5841670000 -0.9636040000
N 1.3604800000 -2.8354280000 -0.2475220000
N -0.2617880000 -2.0994780000 -2.2266130000
H -1.1169580000 -1.6361260000 -2.5627610000
H -0.4634360000 -3.1043590000 -2.1512930000
H 0.4285290000 -2.0037660000 -2.9816870000
H -4.5630370000 -1.3382980000 0.0852790000
H -4.1536700000 0.7841080000 -0.5676740000

[(bpyPy₂Me)Fe(NH₃)(N)]²⁺, multiplicity = 2

C -2.5642120000 2.2289620000 -0.8426820000
C -3.0420920000 0.9360100000 -0.6048370000
C -2.1106790000 -0.0946610000 -0.4288300000
N -0.7787040000 0.1619830000 -0.5505020000
C -0.2928040000 1.4164540000 -0.6266510000
C -1.1865560000 2.4846470000 -0.8047630000
C -3.6849330000 -1.9637010000 0.2759090000
C -2.4004860000 -1.4638680000 0.0237050000
C -3.8233320000 -3.2512580000 0.8071240000
C -2.6733260000 -4.0016330000 1.0784210000
C -1.4199420000 -3.4504540000 0.7887590000
N -1.2825990000 -2.2133850000 0.2767440000
C 1.2188620000 1.5841170000 -0.3539250000
C 1.5840810000 3.0782320000 -0.3209660000
C 2.0536690000 0.8353270000 -1.4089920000
C 1.4801950000 0.9157990000 1.0286560000
N 1.1153700000 -0.3822630000 1.1646490000
C 1.2443280000 -0.9900760000 2.3621960000
C 1.7831530000 -0.3487040000 3.4789920000
C 2.2005700000 0.9783110000 3.3405240000
C 2.0399540000 1.6195450000 2.1051380000
C 3.0432090000 1.4737380000 -2.1740580000
C 3.7834780000 0.7429960000 -3.1091900000
C 3.5134650000 -0.6196170000 -3.2721070000
C 2.5129470000 -1.1949410000 -2.4918250000
N 1.8104040000 -0.4879030000 -1.5730610000
H -3.2664140000 3.0518630000 -1.0036930000
H -4.8180430000 -3.6599750000 1.0065000000
H -2.7313830000 -5.0088920000 1.4987320000
H -0.5080550000 -4.0262780000 0.9648820000
H 0.9946200000 3.6028090000 0.4459670000
H 2.6502490000 3.2150900000 -0.0880600000
H 1.3811330000 3.5462140000 -1.2961940000
H 0.8928590000 -2.0243110000 2.4351730000

H 1.8657060000 -0.8852230000 4.4277910000
 H 2.6366880000 1.5205470000 4.1849730000
 H 2.3469110000 2.6598330000 1.9930130000
 H 3.2378380000 2.5382620000 -2.0436250000
 H 4.5561820000 1.2387130000 -3.7044090000
 H 4.0555980000 -1.2352080000 -3.9945930000
 H 2.2394960000 -2.2466730000 -2.6080520000
 Fe 0.3450420000 -1.4115640000 -0.5815380000
 H -0.8195020000 3.5070640000 -0.8982600000
 N 1.6020970000 -2.8987290000 -0.0884220000
 H 1.4578630000 -3.7514290000 -0.6423240000
 H 1.5375640000 -3.1848910000 0.8968740000
 N -0.1675210000 -2.0361960000 -1.9733660000
 H 2.5831050000 -2.6211640000 -0.2270840000
 H -4.5642680000 -1.3520350000 0.0611380000
 H -4.1137720000 0.7370230000 -0.5352650000

[(bpyPy₂Me)Fe(NH₃)(N)]²⁺, multiplicity = 4

C -2.5306310000 2.2084930000 -0.8929070000
 C -3.0039710000 0.9092510000 -0.6879970000
 C -2.0718670000 -0.1097690000 -0.4571700000
 N -0.7333210000 0.1512720000 -0.4899630000
 C -0.2665190000 1.4156910000 -0.5554370000
 C -1.1587600000 2.4744930000 -0.7848620000
 C -3.6584370000 -2.0139780000 0.1238860000
 C -2.3723640000 -1.4804870000 -0.0373860000
 C -3.8003300000 -3.3138200000 0.6189580000
 C -2.6515240000 -4.0500360000 0.9409290000
 C -1.3962380000 -3.4740540000 0.7363240000
 N -1.2562270000 -2.2149530000 0.2680450000
 C 1.2394990000 1.5994410000 -0.2695590000
 C 1.6037230000 3.0939030000 -0.2573890000
 C 2.0494850000 0.8433140000 -1.3363720000
 C 1.5123480000 0.9502590000 1.1175290000
 N 1.1881350000 -0.3587390000 1.2639410000
 C 1.3453470000 -0.9618040000 2.4634110000
 C 1.8624890000 -0.2961660000 3.5747430000
 C 2.2320040000 1.0446380000 3.4295800000
 C 2.0495860000 1.6744730000 2.1915850000
 C 3.0277010000 1.4662760000 -2.1247150000
 C 3.7179310000 0.7269110000 -3.0923860000
 C 3.4108980000 -0.6271180000 -3.2640710000
 C 2.4296000000 -1.1919190000 -2.4533460000
 N 1.7765040000 -0.4757740000 -1.5033570000
 H -3.2311100000 3.0246940000 -1.0906030000

H -4.7958700000 -3.7471030000 0.7503230000
 H -2.7145140000 -5.0668010000 1.3368200000
 H -0.4837390000 -4.0334540000 0.9515370000
 H 1.0122850000 3.6289380000 0.5007270000
 H 2.6696660000 3.2347140000 -0.0251810000
 H 1.4022660000 3.5486780000 -1.2389940000
 H 1.0380160000 -2.0093770000 2.5347030000
 H 1.9701310000 -0.8268100000 4.5242270000
 H 2.6532170000 1.6043640000 4.2700970000
 H 2.3253450000 2.7227850000 2.0742110000
 H 3.2530250000 2.5241520000 -1.9892090000
 H 4.4822170000 1.2113710000 -3.7075220000
 H 3.9134720000 -1.2440580000 -4.0132980000
 H 2.1288530000 -2.2373710000 -2.5608740000
 Fe 0.4315840000 -1.3871970000 -0.3567750000
 H -0.7947830000 3.4988020000 -0.8693140000
 N 1.6672700000 -2.9420320000 -0.0010600000
 H 2.6526100000 -2.6754600000 -0.1326070000
 N -0.0816540000 -2.2467590000 -1.8904340000
 H -4.5350370000 -1.4151450000 -0.1335820000
 H -4.0748990000 0.6945140000 -0.6842690000
 H 1.6215250000 -3.3093650000 0.9600240000
 H 1.4927740000 -3.7409330000 -0.6239530000

[(bpyPy₂Me)Fe(NH)(NH₂)]²⁺, multiplicity = 4

C -2.5919440000 2.2288220000 -0.9356270000
 C -3.0658410000 0.9388490000 -0.6692960000
 C -2.1288180000 -0.0801260000 -0.4545380000
 N -0.7988540000 0.1789750000 -0.5730700000
 C -0.3267860000 1.4338590000 -0.6612220000
 C -1.2163030000 2.4971760000 -0.8807080000
 C -3.6835930000 -1.9462760000 0.3253920000
 C -2.4082940000 -1.4334300000 0.0561700000
 C -3.7979470000 -3.2144270000 0.9091490000
 C -2.6361870000 -3.9356680000 1.2091110000
 C -1.3911620000 -3.3771510000 0.8973350000
 N -1.2843310000 -2.1568660000 0.3425300000
 C 1.1774340000 1.5878710000 -0.3438020000
 C 1.5527850000 3.0772850000 -0.2738750000
 C 2.0310210000 0.8473640000 -1.3885720000
 C 1.4147700000 0.8818080000 1.0238580000
 N 1.1072010000 -0.4393370000 1.1216790000
 C 1.2894940000 -1.0997890000 2.2869220000
 C 1.7940290000 -0.4712080000 3.4248830000
 C 2.1274950000 0.8839910000 3.3425720000

C 1.9363400000 1.5634320000 2.1326440000
 C 2.9951060000 1.4964990000 -2.1771260000
 C 3.7664650000 0.7580090000 -3.0796400000
 C 3.5619890000 -0.6230780000 -3.1770320000
 C 2.5850260000 -1.2102710000 -2.3771110000
 N 1.8385460000 -0.4873290000 -1.5068030000
 H -3.2977790000 3.0427220000 -1.1245440000
 H -4.7856210000 -3.6313980000 1.1260610000
 H -2.6797510000 -4.9261700000 1.6694380000
 H -0.4522930000 -3.9110220000 1.0718170000
 H 0.9486270000 3.5924770000 0.4880830000
 H 2.6155580000 3.2029770000 -0.0191020000
 H 1.3707880000 3.5641400000 -1.2438920000
 H 1.0269970000 -2.1608460000 2.2871300000
 H 1.9235160000 -1.0440670000 4.3466810000
 H 2.5339140000 1.4154440000 4.2083040000
 H 2.1939560000 2.6203730000 2.0606430000
 H 3.1461790000 2.5724600000 -2.0870410000
 H 4.5190160000 1.2595250000 -3.6955140000
 H 4.1428650000 -1.2461560000 -3.8620690000
 H 2.3750350000 -2.2813050000 -2.4155160000
 Fe 0.3833060000 -1.4108340000 -0.4955710000
 H -0.8544650000 3.5203240000 -0.9888360000
 N 1.3725770000 -2.8022660000 -0.1754280000
 H 2.3247480000 -3.0280780000 0.1555970000
 N -0.2611060000 -2.0465650000 -2.0938740000
 H -0.7331970000 -1.4660410000 -2.7971720000
 H -0.1337480000 -3.0149300000 -2.4055100000
 H -4.5736040000 -1.3603700000 0.0842130000
 H -4.1373600000 0.7382910000 -0.5998530000

[(bpyPy₂Me)Fe(NH)(NH₂)]²⁺, multiplicity = 2

C -2.5864650000 2.2049550000 -0.8193430000
 C -3.0487510000 0.9137370000 -0.5403760000
 C -2.1055790000 -0.1078840000 -0.3698480000
 N -0.7823450000 0.1610990000 -0.5154340000
 C -0.3110440000 1.4115800000 -0.6394430000
 C -1.2101180000 2.4726480000 -0.8295050000
 C -3.6371630000 -2.0044960000 0.3765200000
 C -2.3706570000 -1.4859040000 0.0738270000
 C -3.7359690000 -3.3078130000 0.8774300000
 C -2.5682410000 -4.0595260000 1.0612890000
 C -1.3345040000 -3.4926410000 0.7252490000
 N -1.2401710000 -2.2354000000 0.2501820000
 C 1.2026350000 1.5670820000 -0.3780410000

C 1.5840130000 3.0559470000 -0.3369200000
 C 2.0387060000 0.8077940000 -1.4249050000
 C 1.4352790000 0.8846820000 0.9992510000
 N 1.0592150000 -0.4140240000 1.1292500000
 C 1.1509730000 -1.0345370000 2.3274990000
 C 1.6526020000 -0.3903220000 3.4582850000
 C 2.0824340000 0.9342710000 3.3357010000
 C 1.9671890000 1.5764290000 2.0967370000
 C 3.0056400000 1.4388570000 -2.2227540000
 C 3.7751220000 0.6827770000 -3.1136760000
 C 3.5700610000 -0.6992540000 -3.1897470000
 C 2.5902920000 -1.2716680000 -2.3819270000
 N 1.8411360000 -0.5292960000 -1.5279690000
 H -3.2998650000 3.0186340000 -0.9779510000
 H -4.7153820000 -3.7291880000 1.1212340000
 H -2.6007100000 -5.0795320000 1.4529470000
 H -0.3920980000 -4.0400910000 0.8230850000
 H 0.9963410000 3.5833300000 0.4294070000
 H 2.6517600000 3.1812580000 -0.1037100000
 H 1.3846710000 3.5289600000 -1.3103910000
 H 0.8183180000 -2.0749040000 2.3655080000
 H 1.7061450000 -0.9309360000 4.4067210000
 H 2.4961180000 1.4724110000 4.1937510000
 H 2.2844380000 2.6144010000 1.9923860000
 H 3.1622370000 2.5151850000 -2.1491250000
 H 4.5303680000 1.1728820000 -3.7353120000
 H 4.1541540000 -1.3341420000 -3.8609070000
 H 2.3769510000 -2.3436530000 -2.3977790000
 Fe 0.4106810000 -1.4346240000 -0.5245350000
 H -0.8505920000 3.4937860000 -0.9617860000
 N 1.4607610000 -2.6924620000 -0.0243450000
 H 2.3633930000 -2.5920210000 0.4773750000
 N -0.2770660000 -1.9196490000 -2.1325450000
 H 0.0166770000 -1.4383350000 -2.9907720000
 H -1.2380130000 -2.2680340000 -2.2335960000
 H -4.5307390000 -1.3939320000 0.2274540000
 H -4.1170420000 0.7092350000 -0.4405700000

[(bpyPy₂Me)Fe(NH)(NH₃)]³⁺, multiplicity = 2

C -2.5712280000 2.2178060000 -0.9244260000
 C -3.0404620000 0.9284080000 -0.6477880000
 C -2.1012650000 -0.0852620000 -0.4272160000
 N -0.7705480000 0.1827520000 -0.5421920000
 C -0.3008830000 1.4384110000 -0.6547530000
 C -1.1957630000 2.4919110000 -0.8845300000

C -3.6404530000 -1.9649730000 0.3409270000
C -2.3720780000 -1.4467620000 0.0496240000
C -3.7418760000 -3.2539960000 0.8773340000
C -2.5754500000 -3.9942470000 1.1044650000
C -1.3371510000 -3.4344950000 0.7740110000
N -1.2433500000 -2.1872140000 0.2691490000
C 1.2024080000 1.6004320000 -0.3559550000
C 1.5760260000 3.0896330000 -0.2897540000
C 2.0512150000 0.8559290000 -1.3993340000
C 1.4395390000 0.8939320000 1.0069640000
N 1.0901310000 -0.4136590000 1.1217190000
C 1.2095750000 -1.0691570000 2.3009040000
C 1.7191110000 -0.4396080000 3.4351800000
C 2.1123280000 0.8976740000 3.3382280000
C 1.9656540000 1.5675760000 2.1175620000
C 3.0240870000 1.4969890000 -2.1807580000
C 3.8024400000 0.7539990000 -3.0734640000
C 3.6037640000 -0.6283190000 -3.1627700000
C 2.6207620000 -1.2121900000 -2.3696260000
N 1.8564830000 -0.4799050000 -1.5176300000
H -3.2806960000 3.0277400000 -1.1153540000
H -4.7232360000 -3.6725840000 1.1163780000
H -2.6075080000 -5.0004060000 1.5289180000
H -0.4009170000 -3.9833090000 0.9076010000
H 0.9733160000 3.6033420000 0.4735390000
H 2.6392690000 3.2151110000 -0.0383990000
H 1.3896230000 3.5731950000 -1.2604150000
H 0.8875760000 -2.1126150000 2.3252160000
H 1.8076020000 -1.0057220000 4.3658790000
H 2.5260010000 1.4244310000 4.2029140000
H 2.2539230000 2.6156760000 2.0349680000
H 3.1764320000 2.5726760000 -2.0894920000
H 4.5621340000 1.2526650000 -3.6823840000
H 4.1991890000 -1.2590480000 -3.8278560000
H 2.4350880000 -2.2893450000 -2.4051090000
Fe 0.4349780000 -1.3973700000 -0.4846550000
H -0.8364190000 3.5133510000 -1.0118580000
N 1.3753370000 -2.6806310000 -0.1166570000
H 2.3493850000 -2.9071240000 0.1738350000
N -0.3375670000 -2.0178310000 -2.2341420000
H -1.1797250000 -1.4962890000 -2.5132370000
H -0.5971940000 -3.0119080000 -2.1834890000
H 0.3275570000 -1.9216700000 -3.0134780000
H -4.5331570000 -1.3640010000 0.1543140000
H -4.1105950000 0.7214480000 -0.5781100000

[(bpyPy₂Me)Fe(NH)(NH₃)]³⁺, multiplicity = 4

C -2.5929170000 2.2451530000 -0.9354480000
C -3.0619770000 0.9526910000 -0.6685440000
C -2.1216000000 -0.0597400000 -0.4482420000
N -0.7909410000 0.2088430000 -0.5506700000
C -0.3246110000 1.4637540000 -0.6516240000
C -1.2192660000 2.5195620000 -0.8832730000
C -3.6569570000 -1.9546550000 0.2937580000
C -2.3913700000 -1.4214080000 0.0300680000
C -3.7530760000 -3.2405040000 0.8417350000
C -2.5844050000 -3.9679150000 1.1084160000
C -1.3475000000 -3.3998640000 0.7997490000
N -1.2568460000 -2.1529450000 0.2846040000
C 1.1776710000 1.6209450000 -0.3439570000
C 1.5588170000 3.1081840000 -0.2807380000
C 2.0178410000 0.8714620000 -1.3917500000
C 1.4219550000 0.9150030000 1.0197140000
N 1.1329430000 -0.4127540000 1.1191730000
C 1.3300890000 -1.0917900000 2.2744410000
C 1.8233840000 -0.4598770000 3.4137300000
C 2.1362410000 0.9002770000 3.3377550000
C 1.9365270000 1.5886710000 2.1325170000
C 2.9806480000 1.5058550000 -2.1875150000
C 3.7704900000 0.7514620000 -3.0626920000
C 3.5981800000 -0.6362750000 -3.1137910000
C 2.6249020000 -1.2155790000 -2.3054620000
N 1.8404470000 -0.4716530000 -1.4831720000
H -3.3021360000 3.0546940000 -1.1286400000
H -4.7353850000 -3.6704470000 1.0559960000
H -2.6191290000 -4.9715600000 1.5379250000
H -0.4075030000 -3.9368060000 0.9530270000
H 0.9590770000 3.6265990000 0.4817570000
H 2.6231380000 3.2284530000 -0.0306300000
H 1.3730010000 3.5914460000 -1.2516490000
H 1.0844140000 -2.1566360000 2.2711110000
H 1.9653830000 -1.0387490000 4.3295860000
H 2.5394880000 1.4300240000 4.2056640000
H 2.1840920000 2.6483950000 2.0668480000
H 3.1219680000 2.5848480000 -2.1187050000
H 4.5219160000 1.2469320000 -3.6845250000
H 4.2041720000 -1.2734630000 -3.7628900000
H 2.4554850000 -2.2958290000 -2.3050280000
Fe 0.3914290000 -1.3530260000 -0.4459780000
H -0.8588970000 3.5417510000 -1.0019950000
N 1.3922250000 -2.7875190000 -0.2000910000
H 2.2779590000 -3.2133830000 0.1190460000

N -0.3095100000 -2.0449910000 -2.2145710000
H -1.1055230000 -1.4989100000 -2.5725060000
H -0.6114260000 -3.0248680000 -2.1358590000
H 0.4065770000 -2.0218470000 -2.9528260000
H -4.5538340000 -1.3702650000 0.0774810000
H -4.1322390000 0.7437010000 -0.6065320000

[(bpyPy₂Me)Fe(NH₂)(NH₂)]³⁺, multiplicity = 4

C -2.5651280000 2.2335530000 -0.9511030000
C -3.0440630000 0.9440540000 -0.6874630000
C -2.1113290000 -0.0741810000 -0.4618350000
N -0.7804160000 0.1908020000 -0.5525520000
C -0.3010000000 1.4399560000 -0.6519850000
C -1.1905060000 2.5000320000 -0.8903980000
C -3.6554290000 -1.9619730000 0.2697230000
C -2.3865350000 -1.4313330000 0.0180820000
C -3.7605480000 -3.2408710000 0.8308580000
C -2.5955510000 -3.9620640000 1.1307550000
C -1.3535530000 -3.3976450000 0.8371850000
N -1.2531910000 -2.1609080000 0.2996840000
C 1.2025800000 1.5933220000 -0.3439920000
C 1.5865670000 3.0798940000 -0.2822090000
C 2.0382410000 0.8414180000 -1.3931760000
C 1.4436360000 0.8885710000 1.0202410000
N 1.1268210000 -0.4317570000 1.1216650000
C 1.2863510000 -1.0995050000 2.2890570000
C 1.7909480000 -0.4726970000 3.4266850000
C 2.1455050000 0.8762430000 3.3410280000
C 1.9681890000 1.5597700000 2.1299170000
C 3.0127720000 1.4706160000 -2.1794110000
C 3.7817690000 0.7167560000 -3.0731660000
C 3.5715370000 -0.6638470000 -3.1578000000
C 2.5898900000 -1.2392580000 -2.3564510000
N 1.8375450000 -0.4960070000 -1.5044210000
H -3.2679050000 3.0473560000 -1.1496520000
H -4.7459320000 -3.6699800000 1.0321160000
H -2.6364690000 -4.9589610000 1.5751030000
H -0.4195220000 -3.9334020000 1.0243470000
H 0.9875300000 3.5999950000 0.4797040000
H 2.6507070000 3.1979240000 -0.0306700000
H 1.4037340000 3.5628740000 -1.2538200000
H 0.9971760000 -2.1535600000 2.3060800000
H 1.9030830000 -1.0461720000 4.3500590000
H 2.5568570000 1.4021390000 4.2074120000
H 2.2388580000 2.6133520000 2.0583950000

H 3.1762580000 2.5449760000 -2.0912400000
 H 4.5417600000 1.2077690000 -3.6880300000
 H 4.1534400000 -1.2995430000 -3.8300360000
 H 2.3824020000 -2.3104430000 -2.3913560000
 Fe 0.3818730000 -1.3811050000 -0.4630510000
 H -0.8235760000 3.5199950000 -1.0077450000
 N 1.4570180000 -2.8580050000 -0.1571200000
 H 1.4052930000 -3.7313660000 -0.6980010000
 H 2.2612890000 -2.8647490000 0.4867180000
 N -0.2172930000 -2.0416540000 -2.0852080000
 H -0.8674670000 -2.8338130000 -2.1770260000
 H -0.0062370000 -1.6103970000 -2.9948830000
 H -4.5483600000 -1.3793740000 0.0333010000
 H -4.1159860000 0.7415120000 -0.6321940000

[(bpyPy₂Me)Fe(NH₂)(NH₂)]³⁺, multiplicity = 2

C -2.5498790000 2.2118680000 -0.9257390000
 C -3.0282910000 0.9227650000 -0.6644420000
 C -2.0970270000 -0.0967110000 -0.4410090000
 N -0.7655800000 0.1700770000 -0.5331790000
 C -0.2818320000 1.4215370000 -0.6414390000
 C -1.1737080000 2.4777090000 -0.8744040000
 C -3.6473360000 -1.9713940000 0.2981680000
 C -2.3736380000 -1.4600170000 0.0195170000
 C -3.7616890000 -3.2548950000 0.8440660000
 C -2.5994180000 -3.9899250000 1.1043380000
 C -1.3552510000 -3.4364340000 0.7835410000
 N -1.2444730000 -2.2006980000 0.2549240000
 C 1.2237940000 1.5864970000 -0.3558940000
 C 1.5944500000 3.0762760000 -0.2859440000
 C 2.0582660000 0.8514200000 -1.4173910000
 C 1.4718580000 0.8736280000 1.0005930000
 N 1.1062650000 -0.4312280000 1.1016670000
 C 1.2026420000 -1.0812350000 2.2853740000
 C 1.7202920000 -0.4653810000 3.4238600000
 C 2.1436370000 0.8631010000 3.3291350000
 C 2.0101240000 1.5385520000 2.1092250000
 C 3.0446740000 1.4874480000 -2.1847670000
 C 3.8059330000 0.7438670000 -3.0926030000
 C 3.5749890000 -0.6313340000 -3.2117480000
 C 2.5793940000 -1.2098370000 -2.4297120000
 N 1.8352230000 -0.4767490000 -1.5612820000
 H -3.2530200000 3.0269680000 -1.1180800000
 H -4.7475300000 -3.6697780000 1.0706220000
 H -2.6374150000 -4.9872390000 1.5484680000

H -0.4325250000 -3.9939700000 0.9616140000
 H 0.9972450000 3.5854250000 0.4847500000
 H 2.6591950000 3.2006850000 -0.0403470000
 H 1.4033870000 3.5646720000 -1.2532850000
 H 0.8538720000 -2.1167070000 2.3147900000
 H 1.7850480000 -1.0300940000 4.3572890000
 H 2.5647130000 1.3803670000 4.1960530000
 H 2.3187580000 2.5810220000 2.0295650000
 H 3.2211970000 2.5571960000 -2.0717200000
 H 4.5765020000 1.2372930000 -3.6920880000
 H 4.1543240000 -1.2598460000 -3.8929580000
 H 2.3650960000 -2.2807400000 -2.4816360000
 Fe 0.4097390000 -1.3899000000 -0.5387250000
 H -0.8066660000 3.4969620000 -0.9966260000
 N 1.4669290000 -2.7673260000 -0.0743320000
 H 1.2832920000 -3.7510900000 -0.3225120000
 H 2.3103580000 -2.6752740000 0.5113220000
 N -0.2198610000 -2.0496860000 -2.0866110000
 H -0.9533000000 -2.7698030000 -2.1769200000
 H 0.0554430000 -1.6903170000 -3.0142380000
 H -4.5346560000 -1.3674900000 0.0959480000
 H -4.0999140000 0.7180730000 -0.6130730000

MeCN, multiplicity = 1

C -7.9305190000 -10.7267220000 1.0655210000
 C -6.4737070000 -10.6286630000 1.1098320000
 H -8.2821500000 -11.4458010000 1.8240930000
 H -8.2537290000 -11.0687220000 0.0681850000
 H -8.3795340000 -9.7405370000 1.2700280000
 N -5.3082150000 -10.5499520000 1.1453180000

NH₃, multiplicity = 1

N -3.4062600000 2.0314360000 -0.0471600000
 H -2.3807850000 1.9549480000 0.0223060000
 H -3.6991510000 2.1535560000 0.9330710000
 H -3.6990690000 1.0670120000 -0.2609860000

N₂H₄, multiplicity = 1

N	-5.65593157558449	-0.68732489801612	0.06171968010262
N	-5.58810331553809	0.79856577094464	-0.06171888099823
H	-5.08293721478638	1.08382092202259	0.79073703827746
H	-6.54838235021633	1.09907279415619	0.16372799703163
H	-4.69565325326846	-0.98783209975199	-0.16372998040384

H -6.16110020380625 -0.97258000455531 -0.79073473880964

Ferrocene, multiplicity = 1

C 1.1627240000 0.3769360000 -1.6333370000
C 0.7167690000 -0.9903940000 -1.6334520000
C -0.7212130000 -0.9887400000 -1.6324780000
C -1.1639780000 0.3796340000 -1.6318610000
C 0.0003550000 1.2231080000 -1.6325230000
H 2.2018030000 0.7129070000 -1.6174890000
H 1.3578040000 -1.8747880000 -1.6190580000
H -1.3642490000 -1.8716700000 -1.6173630000
H -2.2022550000 0.7180140000 -1.6147190000
H 0.0016210000 2.3155870000 -1.6151990000
Fe 0.0000100000 -0.0004580000 0.0003460000
C -0.7168910000 -0.9906570000 1.6335370000
C -1.1627810000 0.3767810000 1.6335310000
C -0.0002810000 1.2228930000 1.6328970000
C 1.1640490000 0.3792990000 1.6321590000
C 0.7211570000 -0.9890990000 1.6326470000
H -1.3580070000 -1.8749910000 1.6189140000
H -2.2018330000 0.7128450000 1.6177600000
H -0.0014710000 2.3153770000 1.6157350000
H 2.2023510000 0.7176150000 1.6152970000
H 1.3641030000 -1.8720960000 1.6174310000

Ferrocenium, multiplicity = 2

C 1.0034420000 0.7144730000 -1.7331470000
C 1.0035960000 -0.7133810000 -1.7318490000
C -0.3564340000 -1.1611110000 -1.6909750000
C -1.2040500000 0.0005970000 -1.6691700000
C -0.3563670000 1.1620220000 -1.6928500000
H 1.8888220000 1.3527350000 -1.7038460000
H 1.8891410000 -1.3513810000 -1.7022350000
H -0.6866650000 -2.2006720000 -1.6539200000
H -2.2949760000 0.0008010000 -1.6290140000
H -0.6864970000 2.2016360000 -1.6560550000
Fe -0.0000040000 -0.0000010000 -0.0000120000
C -1.0034430000 -0.7144700000 1.7331380000
C -1.0035920000 0.7133860000 1.7318380000
C 0.3564410000 1.1611120000 1.6909570000
C 1.2040500000 -0.0006030000 1.6691450000
C 0.3563630000 -1.1620260000 1.6928340000
H -1.8888300000 -1.3527250000 1.7039000000
H -1.8891400000 1.3513880000 1.7022790000

H 0.6866770000 2.2006740000 1.6539250000
H 2.2949790000 -0.0008130000 1.6289990000
H 0.6864890000 -2.2016420000 1.6560600000

TEMPO, multiplicity = 2

O -1.2492590000 -0.2906870000 0.4243790000
N -2.4129740000 -0.5340430000 -0.0687860000
C -3.4514420000 0.5490390000 0.1228870000
C -4.6960800000 0.2509660000 -0.7421770000
H -5.5014500000 0.9355480000 -0.4207760000
H -4.4638250000 0.5014720000 -1.7949570000
C -5.1476780000 -1.2107660000 -0.6758460000
H -5.4361800000 -1.4866460000 0.3554200000
H -6.0455870000 -1.3534200000 -1.3025480000
C -4.0144930000 -2.1081980000 -1.1806130000
H -3.7869970000 -1.8351070000 -2.2285590000
H -4.3164130000 -3.1712540000 -1.1859230000
C -2.7198870000 -1.9890100000 -0.3460300000
C -3.8038920000 0.6307340000 1.6263430000
H -2.8760220000 0.7150000000 2.2158510000
H -4.3596980000 -0.2576200000 1.9695330000
H -4.4287020000 1.5213850000 1.8144360000
C -2.8078220000 1.8741840000 -0.3275270000
H -2.5005240000 1.8157310000 -1.3861620000
H -1.9229070000 2.1052830000 0.2851840000
H -3.5423850000 2.6909560000 -0.2199830000
C -2.8390140000 -2.7330520000 1.0051460000
H -1.9496110000 -2.5175820000 1.6208750000
H -2.8942580000 -3.8211660000 0.8270550000
H -3.7387810000 -2.4294760000 1.5664850000
C -1.5302660000 -2.5558200000 -1.1433170000
H -0.6015970000 -2.4934790000 -0.5549750000
H -1.3917840000 -1.9954650000 -2.0842510000
H -1.7274370000 -3.6127590000 -1.3915770000

TEMPOH, multiplicity = 1

O 1.7239200000 0.5195110000 0.6071560000
N 0.5534440000 0.3613860000 -0.2439160000
C -0.4595910000 1.3790490000 0.1817410000
C -1.7239750000 1.1449220000 -0.6810960000
H -2.5119790000 1.8386490000 -0.3351500000
H -1.4870780000 1.4192890000 -1.7271180000

C -2.2101380000 -0.3080670000 -0.6503750000
H -2.5384080000 -0.5847590000 0.3688100000
H -3.0925410000 -0.4249890000 -1.3052220000
C -1.0831280000 -1.2344750000 -1.1182140000
H -0.8361020000 -0.9931040000 -2.1697860000
H -1.3998570000 -2.2935460000 -1.0955690000
C 0.2054860000 -1.0948060000 -0.2712530000
C -0.7963730000 1.3664520000 1.6928030000
H 0.1334780000 1.3495940000 2.2837190000
H -1.4123610000 0.5014020000 1.9846770000
H -1.3576380000 2.2812190000 1.9552670000
C 0.1382480000 2.7576460000 -0.1734590000
H 0.4358270000 2.7807910000 -1.2365620000
H 1.0277660000 2.9682800000 0.4435080000
H -0.6054260000 3.5545730000 0.0045100000
C 0.0393240000 -1.7467730000 1.1238350000
H 0.8885640000 -1.4675830000 1.7693970000
H 0.0283560000 -2.8466450000 1.0207360000
H -0.8953500000 -1.4484380000 1.6253240000
C 1.3640760000 -1.8028180000 -1.0063710000
H 2.2919150000 -1.7559690000 -0.4116310000
H 1.5480220000 -1.3194310000 -1.9820880000
H 1.1147770000 -2.8646390000 -1.1788790000
H 2.4087420000 0.8122760000 -0.0237950000

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